61083

U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

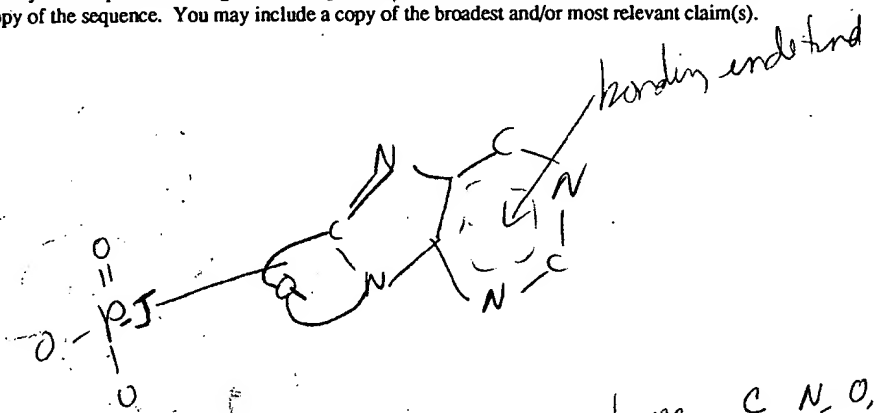
# SEARCH REQUEST FORM

Requestor's Name: BERCH  Serial Number: 09/944086

Date: 2/26/02  Phone: 4718 4D15 4E12  Art Unit: 1624

**Search Topic:**

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevant citations, authors keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevant claim(s).




Q = ~~Bond~~ 1–10 atoms, C, N, O, or S

J = bond or same as Q



**Point of Contact:**
**Susan Hanley**
**Technical Info. Specialist**
**CM1 12C14 Tel: 305-4053**

MARY

4 | 0

**STAFF USE ONLY**

Date completed: 2/28 3/7
Searcher: Hanley
Terminal time:
Elapsed time:
CPU time:
Total time:
Number of Searches:
Number of Databases:

**Search Site**
- STIC
- CM-1
- Pre-S

**Type of Search**
- N.A. Sequence
- A.A. Sequence
- 1 Structure
- Bibliographic

**Vendors**
- IG Suite
- (STN)
- Dialog
- APS
- Geninfo
- SDC
- DARC/Questel
- Other

STR Search

BERCH 09/944,096

```
=> d his

     (FILE 'HOME' ENTERED AT 13:39:02 ON 07 MAR 2002)

     FILE 'REGISTRY' ENTERED AT 13:39:16 ON 07 MAR 2002
               ACT BER096S2/A
              ---------
L1             STR
L2   (      1343)SEA FILE=REGISTRY SSS FUL L1
L3             STR
L4           142 SEA FILE=REGISTRY SUB=L2 SSS FUL L3
              ---------
L5             8 S L4 AND NR=3
L6           134 S L4 NOT L5

     FILE 'HCAPLUS' ENTERED AT 13:39:49 ON 07 MAR 2002
L7             3 S L5
L8            94 S L6
```

1343 cpds from full file search

142 cps from subset search based on L2

8 cpds from L4 have only 3 rings

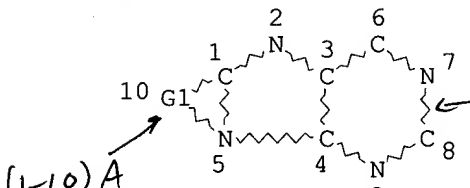
134 cpds have at least one more fused ring

3 cites

94 cites

```
=> d que l7
L1                  STR
```

parent search




all bonding undef.ned

(1-10) A

any nonhydrogen atom

```
REP G1=(1-10) A
NODE ATTRIBUTES:
CONNECT IS E3  RC AT   3
CONNECT IS E3  RC AT   4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L2  (      1343)SEA FILE=REGISTRY SSS FUL L1
L3                  STR
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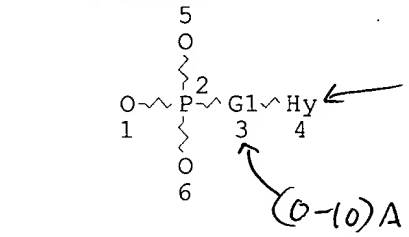
subset search




ring system from L1

(0-10) A

```
REP G1=(0-10) A
NODE ATTRIBUTES:
CONNECT IS E1  RC AT   5
DEFAULT MLEVEL IS ATOM
GGCAT   IS PCY  UNS  AT   4
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS M4 N  AT   4

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   6

STEREO ATTRIBUTES: NONE
L4          142 SEA FILE=REGISTRY SUB=L2 SSS FUL L3
L5            8 SEA FILE=REGISTRY ABB=ON  PLU=ON  L4 AND NR=3
L7            3 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L5
```

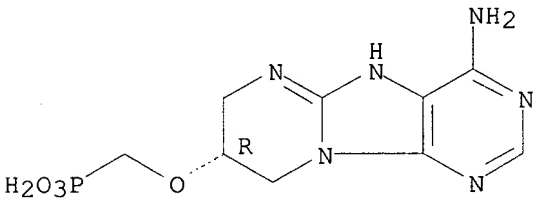
=> d ibib abs hitstr 1

L7 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:379500 HCAPLUS
DOCUMENT NUMBER: 135:137669
TITLE: Synthesis of 8-amino- and N-substituted 8-aminoadenine derivatives of acyclic nucleoside and nucleotide analogs
AUTHOR(S): Janeba, Zlatko; Holy, Antonin; Masojidkova, Milena
CORPORATE SOURCE: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 166 10/6, Czech Rep.
SOURCE: Collection of Czechoslovak Chemical Communications (2001), 66(3), 517-532
CODEN: CCCCAK; ISSN: 0010-0765
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 8-Aminoadenine derivs. were obtained from 8-bromoadenines in one-pot reaction via 8-azidoadenines. Reaction of 8-bromoadenines with methylamine or dimethylamine in ethanol afforded the corresponding N9-substituted 8-(methylamino)adenines and 8-(dimethylamino)adenines. Alkylation of 8-aminoadenine with diverse alkylation agents afforded N9-substituted 8-aminoadenine derivs., and alkylation of 8-(dimethylamino)adenine gave mixts. of the corresponding N9-substituted 8-(dimethylamino)adenines and their N3-substituted regioisomers.

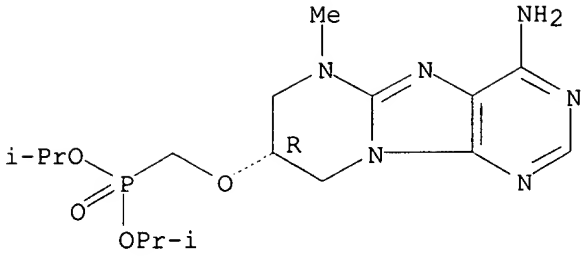
IT **352227-22-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 8-amino- and N-substituted 8-aminoadenine derivs. of acyclic nucleoside and nucleotide analogs via amination and alkylation reactions)
RN 352227-22-6 HCAPLUS
CN Phosphonic acid, [[[(8R)-4-amino-5,7,8,9-tetrahydropyrimido[1,2-e]purin-8-yl]oxy]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



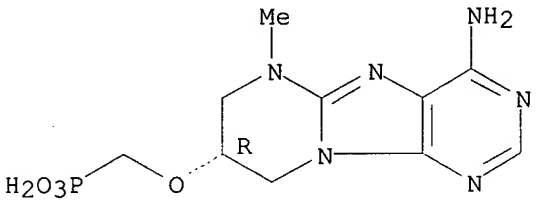

IT **352227-21-5P 352227-23-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of 8-amino- and N-substituted 8-aminoadenine derivs. of acyclic nucleoside and nucleotide analogs via amination and alkylation reactions)
RN 352227-21-5 HCAPLUS
CN Phosphonic acid, [[[(8R)-4-amino-6,7,8,9-tetrahydro-6-methylpyrimido[1,2-e]purin-8-yl]oxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 352227-23-7 HCAPLUS
CN Phosphonic acid, [[[(8R)-4-amino-6,7,8,9-tetrahydro-6-methylpyrimido[1,2-e]purin-8-yl]oxy]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2

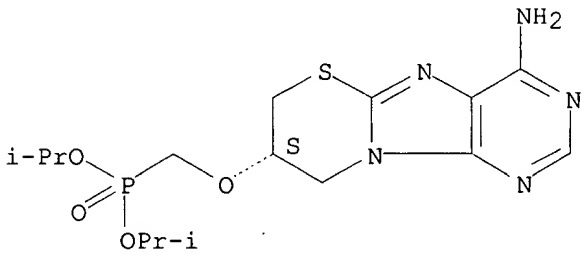
L7 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:61458 HCAPLUS
DOCUMENT NUMBER: 134:208047
TITLE: Synthesis of acyclic nucleoside and nucleotide analogs derived from 6-amino-7H-purine-8(9H)-thione and 8-(methylsulfanyl)adenine
AUTHOR(S): Janeba, Zlatko; Holy, Antonin; Masojidkova, Milena
CORPORATE SOURCE: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.
SOURCE: Collect. Czech. Chem. Commun. (2000), 65(11), 1698-1712
CODEN: CCCCAK; ISSN: 0010-0765
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reaction of 8-bromoadenine derivs. with thiourea in ethanol or butanol was used for the synthesis of the corresponding N9-substituted 6-amino-7H-purine-8(9H)-thiones. 8-(Methylsulfanyl)adenine derivs. were prepd. by reaction of thiones with iodomethane in 1 M sodium methoxide or in aq. 1.5 M potassium hydroxide. Alkylation of 6-amino-7H-purine-8(9H)-thione proceeds preferentially on the sulfur atom. Under similar conditions, alkylation of 8-(methylsulfanyl)adenine with diverse alkylation agents afforded N9-substituted adenine derivs. and N3-substituted adenine derivs. 8,3'-S-Anhydro nucleosides were prepd. in good yields by cyclization of 6-amino-7H-purine-8(9H)-thiones under the Mitsunobu reaction conditions.

IT **328381-27-7P 328381-30-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of acyclic nucleoside and nucleotide analogs derived from aminopurinethione and methylsulfanyladenine)

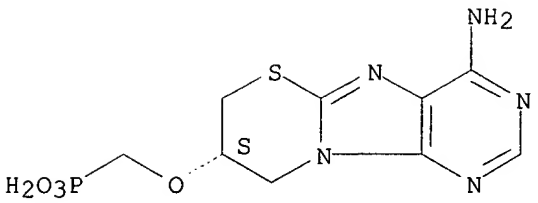
RN 328381-27-7 HCAPLUS
CN Phosphonic acid, [[[(8S)-4-amino-8,9-dihydro-7H-[1,3]thiazino[3,2-e]purin-8-yl]oxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 328381-30-2 HCAPLUS
CN Phosphonic acid, [[[(8S)-4-amino-8,9-dihydro-7H-[1,3]thiazino[3,2-e]purin-8-yl]oxy]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

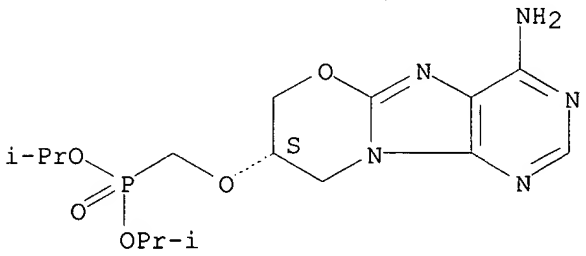
=> d ibib abs hitstr 3

L7 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:617914 HCAPLUS
DOCUMENT NUMBER: 133:322098
TITLE: Synthesis of acyclic nucleoside and nucleotide analogs derived from 6-amino-7H-purin-8(9H)-one
AUTHOR(S): Janeba, Zlatko; Holy, Antonin; Masojidkova, Milena
CORPORATE SOURCE: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 166 10/6, Czech Rep.
SOURCE: Collection of Czechoslovak Chemical Communications (2000), 65(7), 1126-1144
CODEN: CCCCAK; ISSN: 0010-0765
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:322098

AB Reaction of 8-bromoadenine derivs. with sodium acetate in acetic acid and cleavage of (S)-7-[(trityloxy)methyl]-7,8-dihydro[1,3]oxazolo[3,2-e]purin-4-amine and diisopropyl (S)-{[(4-amino-8,9-dihydro-7H-[1,3]oxazino[3,2-e]purin-8-yl)oxy]methyl}phosphonate were used for the synthesis of the corresponding N9-substituted derivs. of 6-amino-7H-purin-8(9H)-one. Alkylation of 6-amino-7H-purin-8(9H)-one with diverse alkylation agents afforded the title N9-monosubstituted and N7,N9-disubstituted acyclic nucleoside and nucleotide analogs.

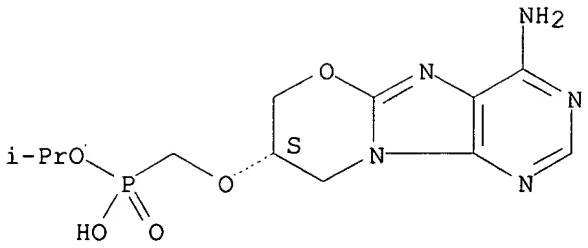
IT **303014-76-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(synthesis of acyclic nucleoside and nucleotide analogs derived from aminopurinone)
RN 303014-76-8 HCAPLUS
CN Phosphonic acid, [[[(8S)-4-amino-8,9-dihydro-7H-[1,3]oxazino[3,2-e]purin-8-yl]oxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



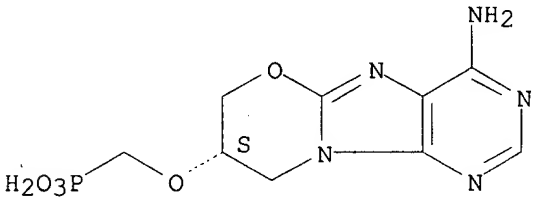

IT **303014-77-9P 303014-85-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of acyclic nucleoside and nucleotide analogs derived from aminopurinone)
RN 303014-77-9 HCAPLUS
CN Phosphonic acid, [[[(8S)-4-amino-8,9-dihydro-7H-[1,3]oxazino[3,2-e]purin-8-yl]oxy]methyl]-, mono(1-methylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 303014-85-9 HCAPLUS
CN Phosphonic acid, [[[(8S)-4-amino-8,9-dihydro-7H-[1,3]oxazino[3,2-e]purin-8-yl]oxy]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 1-20

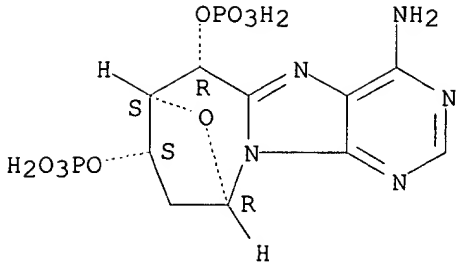
L8 ANSWER 1 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:270326 HCAPLUS
DOCUMENT NUMBER: 133:172961
TITLE: Removal of oxygen free-radical-induced 5',8-purine cyclodeoxynucleosides from DNA by the nucleotide excision-repair pathway in human cells
AUTHOR(S): Kuraoka, Isao; Bender, Christina; Romieu, Anthony; Cadet, Jean; Wood, Richard D.; Lindahl, Tomas
CORPORATE SOURCE: Imperial Cancer Research Fund, Clare Hall Laboratories, South Mimms, EN6 3LD, UK
SOURCE: Proc. Natl. Acad. Sci. U. S. A. (2000), 97(8), 3832-3837
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Exposure of cellular DNA to reactive oxygen species generates several classes of base lesions, many of which are removed by the base excision-repair pathway. However, the lesions include purine cyclodeoxynucleoside formation by intramol. crosslinking between the C-8 position of adenine or guanine and the 5' position of 2-deoxyribose. This distorting form of DNA damage, in which the purine is attached by two covalent bonds to the sugar-phosphate backbone, occurs as distinct diastereoisomers. It was obsd. here that both diastereoisomers block primer extension by mammalian and microbial replicative DNA polymerases, using DNA with a site-specific purine cyclodeoxynucleoside residue as template, and consequently appear to be cytotoxic lesions. Plasmid DNA contg. either the 5'R or 5'S form of 5',8-cyclo-2-deoxyadenosine was a substrate for the human nucleotide excision-repair enzyme complex. The R diastereoisomer was more efficiently repaired than the S isomer. No correction of the lesion by direct damage reversal or base excision repair was detected. Dual incision around the lesion depended on the core nucleotide excision-repair protein XPA. In contrast to several other types of oxidative DNA damage, purine cyclodeoxynucleosides are chem. stable and would be expected to accumulate at a slow rate over many years in the DNA of nonregenerating cells from xeroderma pigmentosum patients. High levels of this form of DNA damage might explain the progressive neurodegeneration seen in XPA individuals.

IT **288404-75-1 288404-76-2 288404-77-3**
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BIOL (Biological study); PROC (Process)
(removal of oxygen free-radical-induced 5',8-purine cyclodeoxynucleosides from DNA by nucleotide excision-repair pathway in human cells)

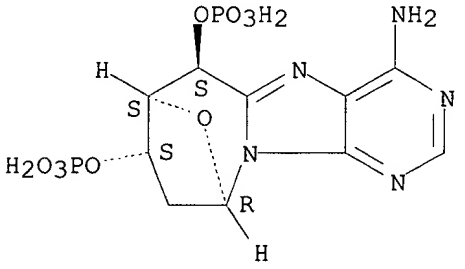
RN 288404-75-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8-diol, 4-amino-7,8,9,10-tetrahydro-, bis(dihydrogen phosphate) (ester), (6R,7S,8S,10R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



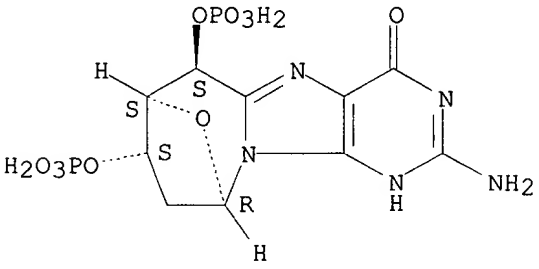
RN 288404-76-2 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8-diol, 4-amino-7,8,9,10-tetrahydro-, bis(dihydrogen phosphate) (ester), (6S,7S,8S,10R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 288404-77-3 HCAPLUS
CN 7,10-Epoxy-4H-azepino[1,2-e]purin-4-one, 2-amino-1,6,7,8,9,10-hexahydro-6,8-bis(phosphonooxy)-, (6S,7S,8S,10R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:213880 HCAPLUS
DOCUMENT NUMBER: 133:17732
TITLE: The synthesis of cyclo-nucleotides with fixed glycosidic bond linkages as putative agonists for P2-purinergic receptors
AUTHOR(S): Tusa, Girolamo; Reed, Juta K.
CORPORATE SOURCE: Department of Chemistry, University of Toronto at

Mississauga, Mississauga, ON, L5L 1C6, Can.
SOURCE: Nucleosides, Nucleotides Nucleic Acids (2000), 19(4), 805-813
CODEN: NNNAFY; ISSN: 1525-7770
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

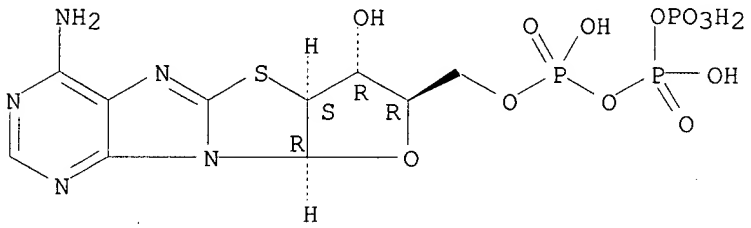
AB Cyclo-nucleotides with fixed glycosidic bond linkages were investigated as possible ligands for purinoceptors in PC12 cells. P2Y2-purinoceptors were not activated by the ATP analog, 8,2'-thioanhydroadenosine-5'-triphosphate and only weakly by the UTP analog, 2,2'-anhydrouridine-5'-triphosphate. However, both analogs were agonists for P2X2-purinoceptors although the potencies were approx. 30-fold less than that of the parent nucleotides.

IT **272108-15-3P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of cyclo-nucleotides with fixed glycosidic bond linkages as putative agonists for P2-purinergic receptors)

RN 272108-15-3 HCAPLUS

CN Triphosphoric acid, P-[[(6aS,7R,8R,9aR)-4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester, tetrasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.




●4 Na

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:583221 HCAPLUS
DOCUMENT NUMBER: 131:214518

TITLE: Method for preparation of 8-(glycosyloxy)purine nucleoside derivatives by glycosylation of 8-substituted purine nucleoside

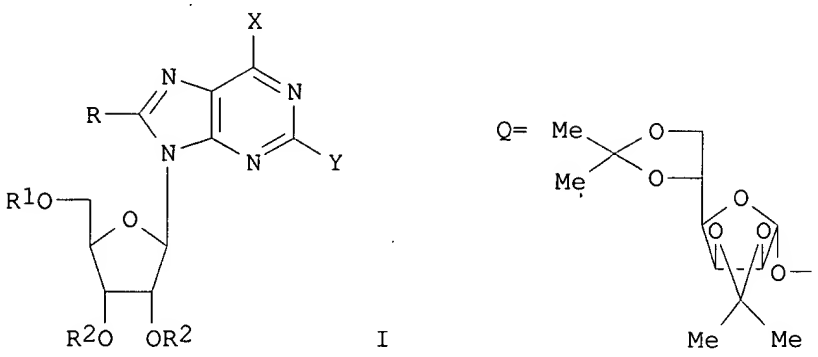
INVENTOR(S): Sugimura, Hideyuki; Satnsfield, Kevin
PATENT ASSIGNEE(S): Noguchi Research Institute, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 11246591 | A2 | 19990914 | JP 1998-66263 | 19980302 |

OTHER SOURCE(S): CASREACT 131:214518; MARPAT 131:214518

GI



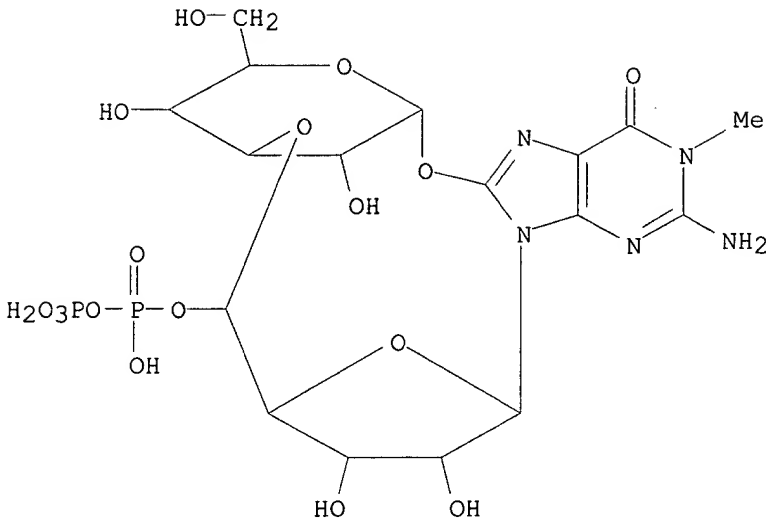

I

AB The title compds. (I; R = HO-protected glycofuranosyloxy or glycopyranosyloxy; X = protected NH2 or OH; Y = H, protected NH2; R1 = HO-protecting group such as triarylmethyl or acetal), which are useful as intermediates for guanofosfocins (chitin synthase inhibitors), are prepd. by reaction of 8-substituted purine nucleosides (I; R = halo, alkyl or arylsulfonyl; R1, R2, X, Y = same as above) with 1-alkoxide of HO-protected glucofuranose or glucopyranose or glycosylation of 8-hydroxypurine nucleosides (I; R = OH; R1, R2, X, Y = same as above) in org. solvent. Thus, 24 mg 2,3:5,6-di-isopropylidene-.alpha.-D-mannofuranose was dissolved in 2 mL DMF and treated with 3.5 mg NaH (60%) for 15 min, followed by adding 36 mg 8-bromo-2',3'-O-isopropylidene-5'-O-dimethoxytrityl-N6-benzoyladenosine, and the resulting mixt. was allowed to react at room temp. for 6 h to give, after silica gel chromatog., 71% I (R = Q, X = NHBz, Y = H, R1 = dimethoxytrityl, R2R2 = CMe2).

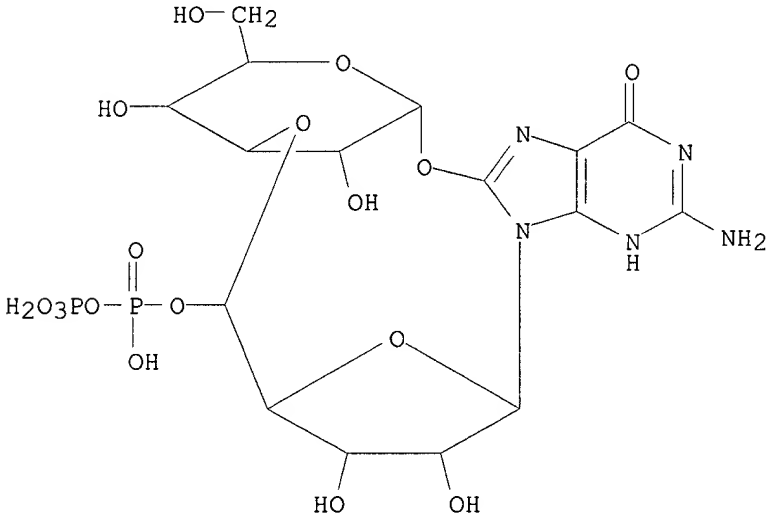
IT **183658-78-8P**, Guanofosfocin A **183658-79-9P**, Guanofosfocin B **183658-80-2P**, Guanofosfocin C
RL: PNU (Preparation, unclassified); PREP (Preparation)
(prepn. of 8-(glycosyloxy)purine nucleoside derivs. as intermediates for guanofosfocins by glycosylation of 8-substituted purine nucleoside)

RN 183658-78-8 HCAPLUS

CN Diphosphoric acid, mono[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-2-amino-3,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-3-methyl-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-13-yl] ester (9CI) (CA INDEX NAME)

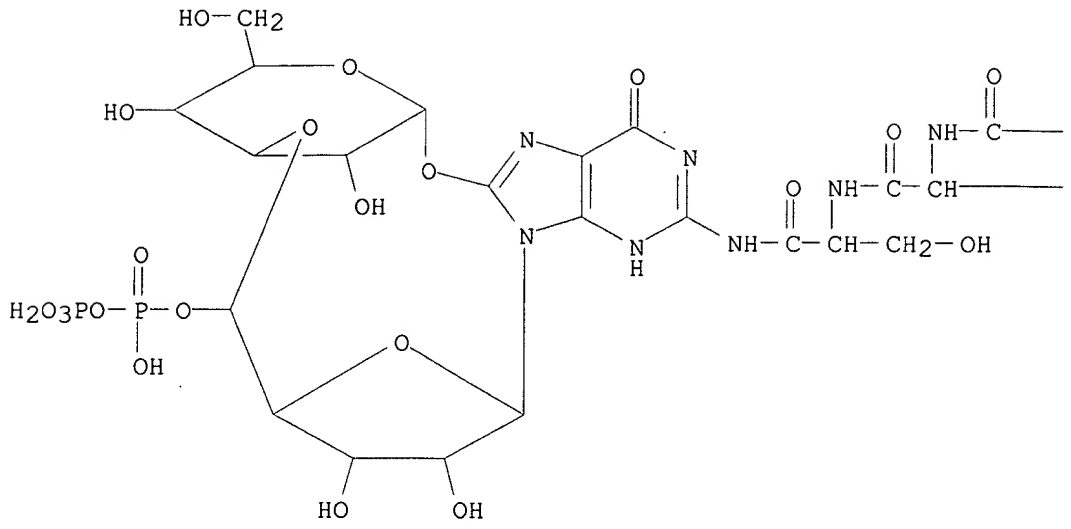


RN 183658-79-9 HCAPLUS
CN Diphosphoric acid, mono[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-2-amino-1,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-13-yl] ester (9CI) (CA INDEX NAME)

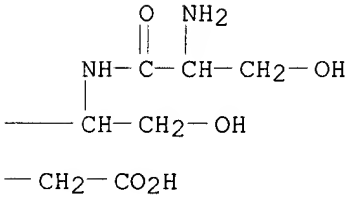


RN 183658-80-2 HCAPLUS
CN L-Serinamide, L-seryl-L-seryl-L-.alpha.-aspartyl-N-[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-1,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-13-[[hydroxy(phosphonooxy)phosphinyl]oxy]-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



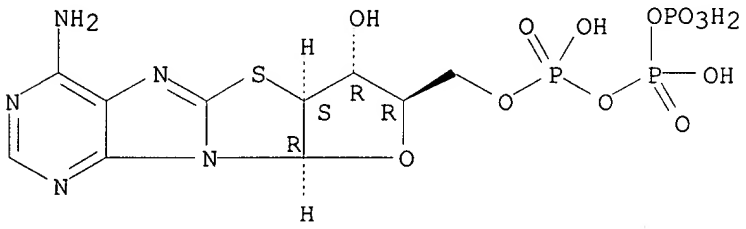
L8 ANSWER 4 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:363009 HCAPLUS
DOCUMENT NUMBER: 131:182753
TITLE: The effects of various GTP analogues on microtubule assembly
AUTHOR(S): Muraoka, Masako; Fukuzawa, Hiromi; Nishida, Akiko; Okano, Kyoko; Tsuchihara, Tomoko; Shimoda, Asako; Suzuki, Yuko; Sato, Mamiko; Osumi, Masako; Sakai, Hikoichi
CORPORATE SOURCE: Department of Chemical and Biological Sciences, Faculty of Science, Japan Women's University, Tokyo, 112-8681, Japan
SOURCE: Cell Struct. Funct. (1999), 24(2), 101-109
CODEN: CSFUDY; ISSN: 0386-7196
PUBLISHER: Japan Society for Cell Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We synthesized 27 GTP analogs with modification or substitution at positions C2, C6, C8 and ribose moiety to investigate their effect on microtubule (Mt) assembly. It was found that C2 and C6 are both functional for the analogs supporting Mt assembly. It was surprising to find that 2-amino-ATP (n2ATP) substantially supports assembly, and that

the appearance of the assembled Mts was indistinguishable from those assembled in the std. GTP assembly buffer soln. Furthermore, 2-amino dATP and dGTP are even more potent than GTP in supporting assembly. The substitution of oxo group at C6 with reactive thiol largely reduced the activity of the analog to support assembly. When free rotation of the glycosidic linkage of GTP was blocked by the introduction of sulfur atom between C8 and C2' of ribose moiety, it resulted in total suppression of assembly. Purine nucleoside triphosphate was found to support assembly better than GTP, and even more efficient was 2-amino purine nucleoside triphosphate. Interestingly, their deoxy-type analogs were totally inhibitory. Although 2-amino 8-hydroxy ATP and other analogs supported assembly much better than did GTP, their diphosphate analogs were totally incapable of supporting assembly. Finally, bulky fluorescent probes were introduced at C3' of ribose moiety (Mant-8-Br-GTP or Mant-GTP) to visualize the fluorescent signal in assembled Mts. Even in this case, the no. of most protofilaments was found to be 14, consistent with that found in Mts assembled in GTP std. buffer soln.

IT **68745-46-0 240126-68-5 240126-69-6**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(effects of various GTP analogs on microtubule assembly)

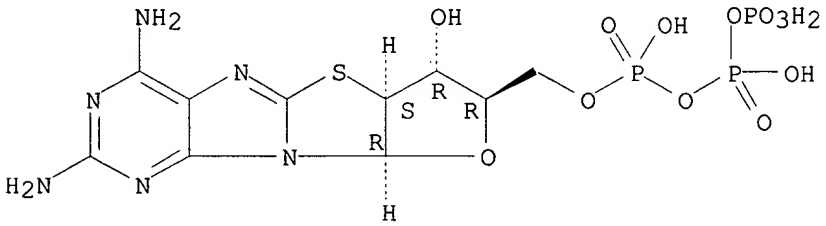
RN 68745-46-0 HCAPLUS
CN Triphosphoric acid, P-[[(6aS,7R,8R,9aR)-4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



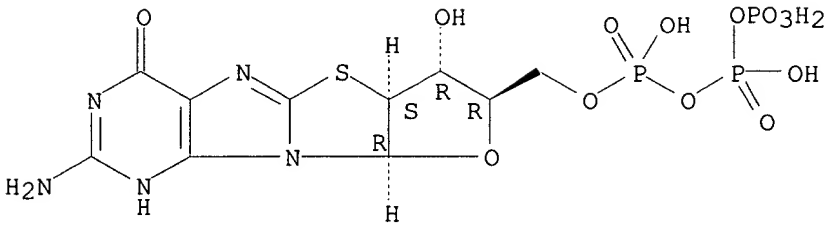
RN 240126-68-5 HCAPLUS
CN Triphosphoric acid, P-[[(6aS,7R,8R,9aR)-2,4-diamino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 240126-69-6 HCAPLUS
CN Triphosphoric acid, P-[[(6aS,7R,8R,9aR)-2-amino-1,4,6a,7,8,9a-hexahydro-7-hydroxy-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

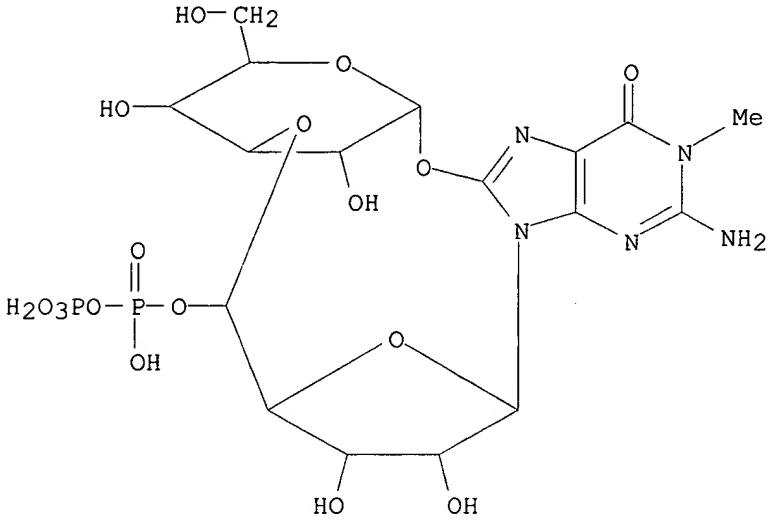
L8 ANSWER 5 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:313239 HCAPLUS
DOCUMENT NUMBER: 131:73906
TITLE: Synthetic studies on guanofosfocins - synthesis of 8-(mannopyranosyloxy)adenosine derivatives
AUTHOR(S): Sugimura, Hideyuki; Kanamori, Hideyuki; Stansfield, Kevin
CORPORATE SOURCE: Noguchi Institute, Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1998), 40th, 655-660
CODEN: TYKYDS
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

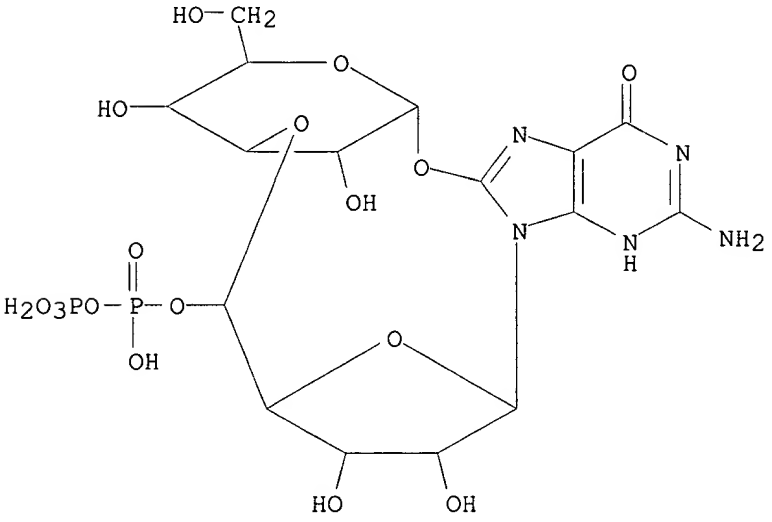
AB Two approaches for the synthesis of 8-(glycosyloxy)purine nucleoside, which is found in a recently isolated chitin synthase inhibitor-guanofosfocin, have been examd. One contains substitution reaction of alc. with purine nucleoside bearing a leaving group at the 8 position. Through a no. of model reactions using cyclohexanol as a nucleophile and 8-substituted adenosine derivs. as a substrate, we finally found that N6-benzoyl-8-bromoadenosine deriv. (I; R = Br, R1 = Bz, R2 = 4,4'-dimethoxytrityl) reacted with sodium alkoxides derived from di-O-isopropylidene-.alpha.-D-mannoses (Q-H and Q1-H), in DMF at room temp. to yield 8-(mannosyloxy)adenosines (I; R = Q, R1 = Bz) and (I; R = Q1, R1 = Bz) and in reasonable yields. Another approach involves glycosylation reaction of 8-oxoadenosine derivs. with appropriate mannosyl donors. We found that N6-trityl-adenosine deriv. (II) was a suitable substrate for this reaction. When 2,3,4,6-tetra-O-benzyl-.alpha.-D-mannosyl bromide was allowed to react with 8-hydroxyadenosine deriv. (II) in the presence of silver carbonate in toluene at 60.degree.C, 8-(mannosyloxy)adenosine (I; R = Q2, R1 = R2 = Tr) is obtained in 79% yield. The 8-mannosyloxy products were isolated solely as .alpha. anomers, assigned by 1JC-H value of C-1 in the mannose moiety.

IT **183658-78-8P**, Guanofosfocin A **183658-79-9P**, Guanofosfocin B **183658-80-2P**, Guanofosfocin C
RL: PNU (Preparation, unclassified); PREP (Preparation)
(prepn. of 8-(mannopyranosyloxy)adenosine derivs. as intermediates for guanofosfocins)

RN 183658-78-8 HCAPLUS
CN Diphosphoric acid, mono[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-2-amino-3,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-3-methyl-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-13-yl] ester (9CI) (CA INDEX NAME)



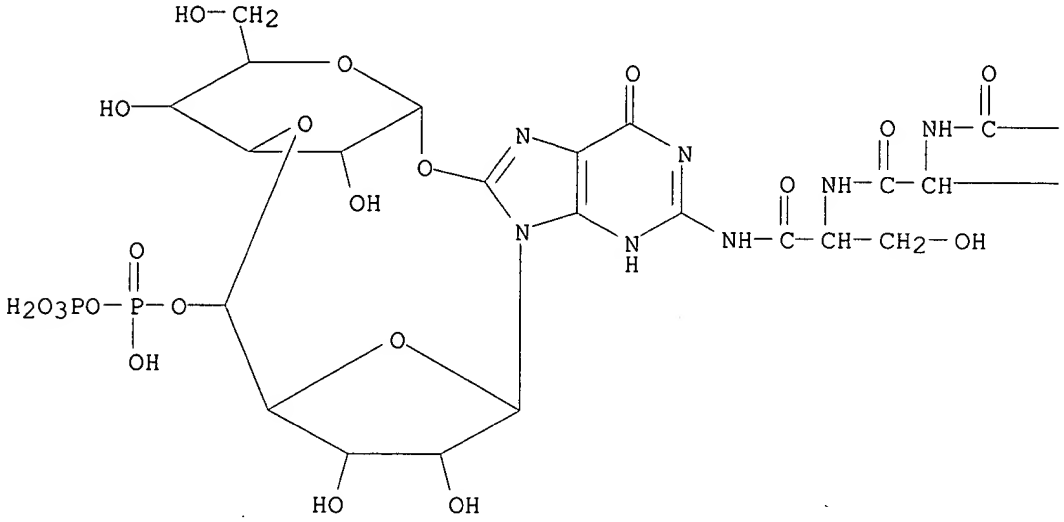
RN 183658-79-9 HCAPLUS
CN Diphosphoric acid, mono[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-2-amino-1,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-13-yl] ester (9CI) (CA INDEX NAME)



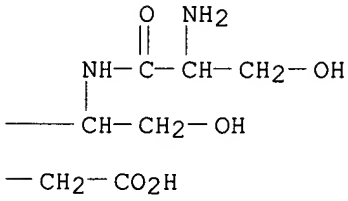
RN 183658-80-2 HCAPLUS
CN L-Serinamide, L-seryl-L-seryl-L-.alpha.-aspartyl-N-[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-1,4,10,11,14,15,16,17-octahydro-

10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-13-[[hydroxy(phosphonooxy)phosphinyl]oxy]-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



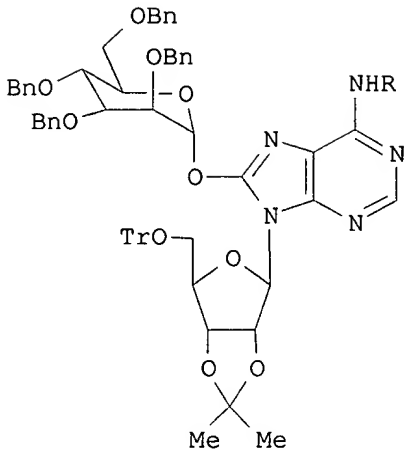
PAGE 1-B



L8 ANSWER 6 OF 94 HCAPLUS COPYRIGHT 2002 ACS

| | |
|---|---|
| ACCESSION NUMBER: | 1998:605258 HCAPLUS |
| DOCUMENT NUMBER: | 129:316496 |
| TITLE: | Synthesis of 8-(mannosyloxy)adenosine. A novel nucleoside-carbohydrate hybrid |
| AUTHOR(S): | Sugimura, Hideyuki; Stansfield, Kevin |
| CORPORATE SOURCE: | Noguchi Inst., Tokyo, 173, Japan |
| SOURCE: | Synlett (1998), (9), 985-986<br>CODEN: SYNLES; ISSN: 0936-5214 |
| PUBLISHER: | Georg Thieme Verlag |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |

GI



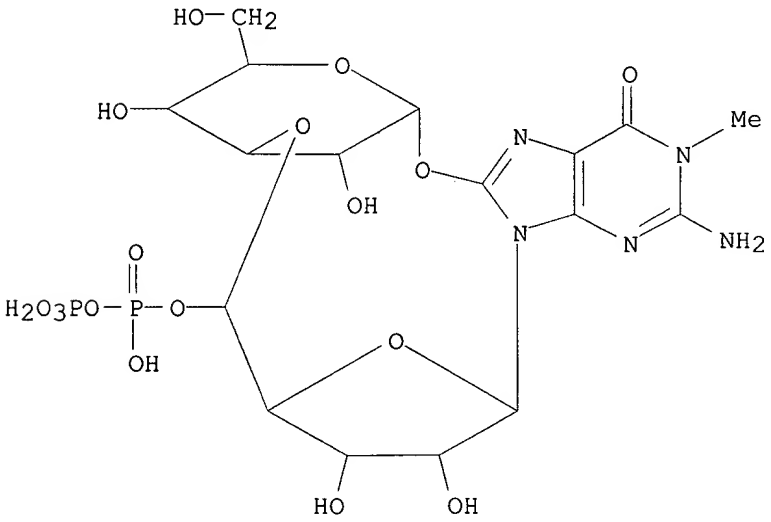
I

AB As a basic study directed towards the synthesis of guanofosfocin analogs, the nucleoside-carbohydrate hybrid I (Bn = PhCH2; Tr = Ph3C; R = PhCO, Ph3C) was prepd. by glycosylation of 8-oxoadenosines with mannopyranosyl bromide in the presence of Ag2CO3.

IT **183658-78-8P**, Guanofosfocin A
RL: PNU (Preparation, unclassified); PREP (Preparation)
(prepn. of (mannosyloxy)adenosine as guanofosfocin precursor)

RN 183658-78-8 HCAPLUS

CN Diphosphoric acid, mono[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-2-amino-3,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-3-methyl-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-13-yl] ester (9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:446898 HCAPLUS
DOCUMENT NUMBER: 129:203192
TITLE: Site-Specific Introduction of (5'S)-5',8-Cyclo-2'-

deoxyadenosine into Oligodeoxyribonucleotides

AUTHOR(S): Romieu, Anthony; Gasparutto, Didier; Molko, Didier; Cadet, Jean

CORPORATE SOURCE: Departement de Recherche Fondamentale sur la Matiere Condensee SCIB/Laboratoire des lesions des Acides Nucleiques, CEA Grenoble, Grenoble, F-38054, Fr.

SOURCE: J. Org. Chem. (1998), 63(15), 5245-5249
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis provided herein provides a facile method for the prepn. of oligonucleotides contg. (5'S)-CyclodAdo at specific positions. We also demonstrate the high stability of phosphodiester linkages, between (5'S)-CyclodAdo and normal 3'-deoxyribonucleosides, toward the enzymic hydrolysis and that the (5'S)-CycloA-T base pair is less stable than the A-T base pair. These modified DNA fragments are suitable for further studies aimed at detg. both the biochem. and conformational features of (5'S)-CyclodAdo into DNA fragments.

IT **211919-92-5P 211919-93-6P**

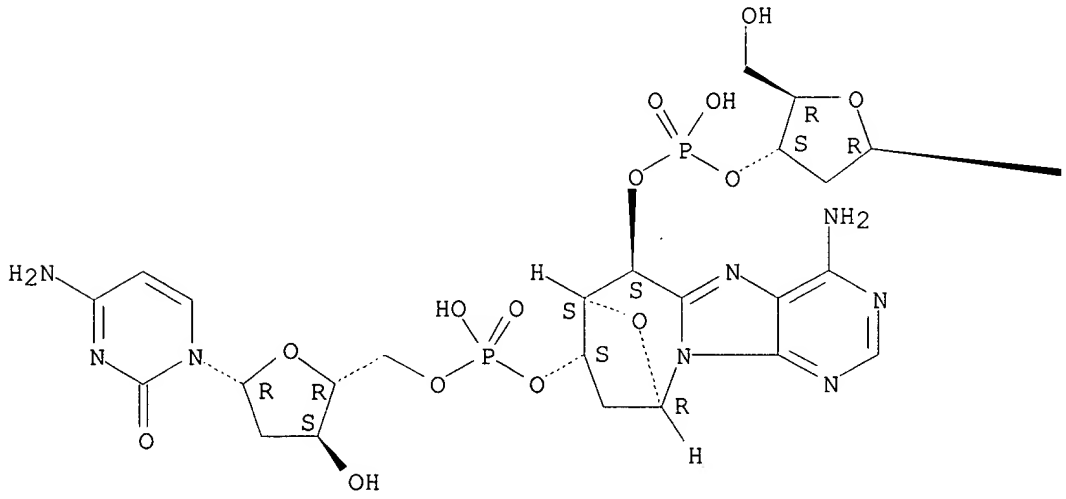
RL: SPN (Synthetic preparation); PREP (Preparation)
(site-specific introduction of (5'S)-cyclodeoxyadenosine into oligodeoxyribonucleotides)

RN 211919-92-5 HCAPLUS

CN Cytidine, 2'-deoxyguanylyl-(3'.fwdarw.5')-(5'S)-2'-deoxy-5',8-C-cycloadenylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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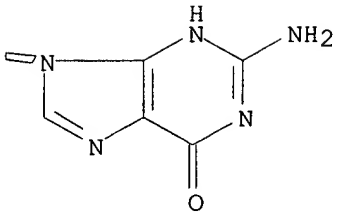
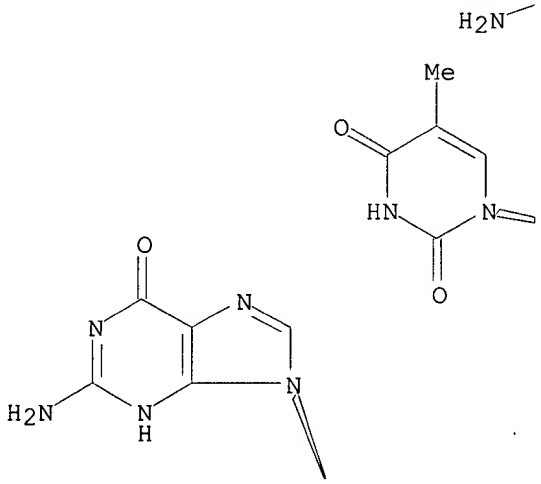


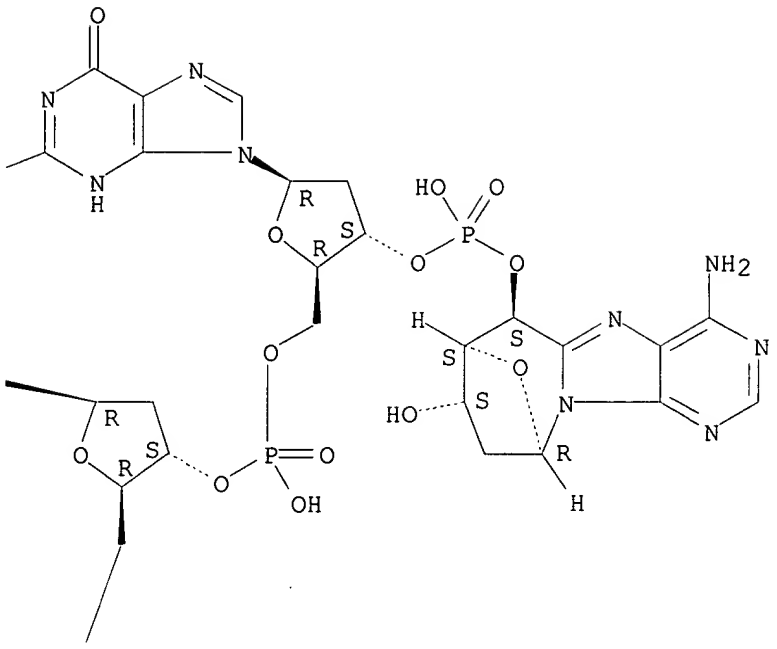
RN 211919-93-6 HCAPLUS
CN 5',8-C-Cycloadenosine, 2'-deoxyadenylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2'-deoxycytidylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2'-deoxy-, (5'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

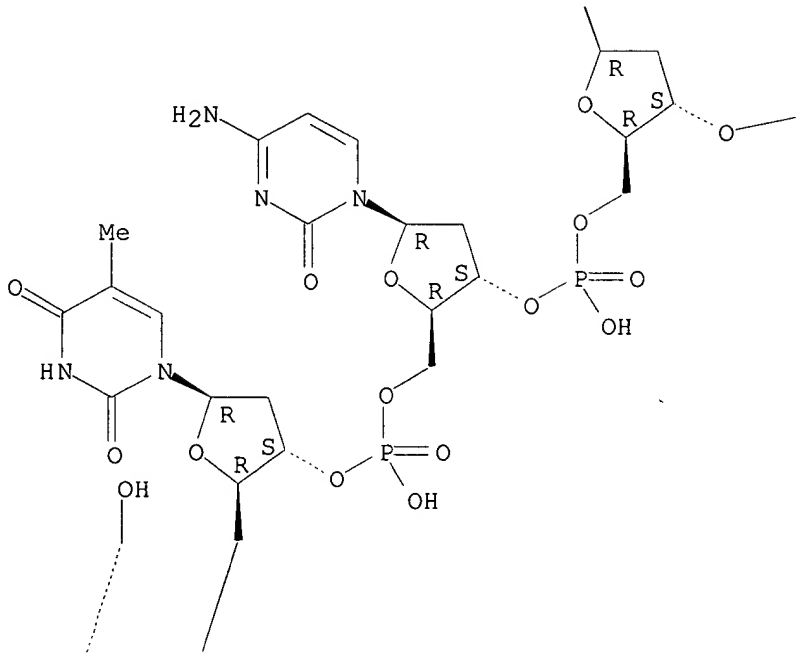
PAGE 1-A



PAGE 1-B



PAGE 2-A



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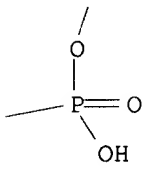

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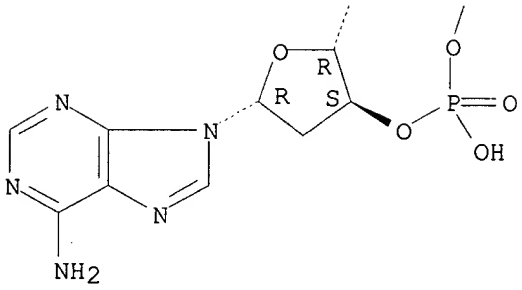
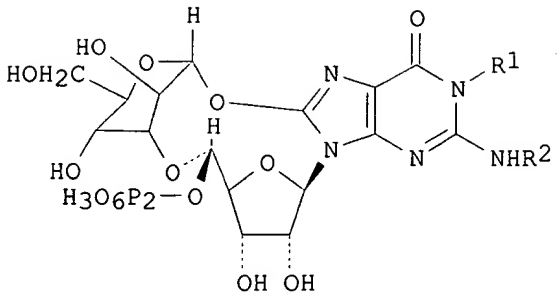


L8 ANSWER 8 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:703669 HCAPLUS
DOCUMENT NUMBER: 125:322575
TITLE: Isolation and structure elucidation of novel chitin synthase inhibitors guanofosfocins produced by microorganisms
AUTHOR(S): Katoh, H.; Yamada, M.; Lida, K.; Aoki, M.; Itezono, Y.; Nakayama, N.; Suzuki, Y.; Watanabe, M.; Shimada, H.; et al.
CORPORATE SOURCE: Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1996), 38th, 115-120
CODEN: TYKYDS
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I R 1 = Me, R2 = H

II R 1 = H, R2 = H

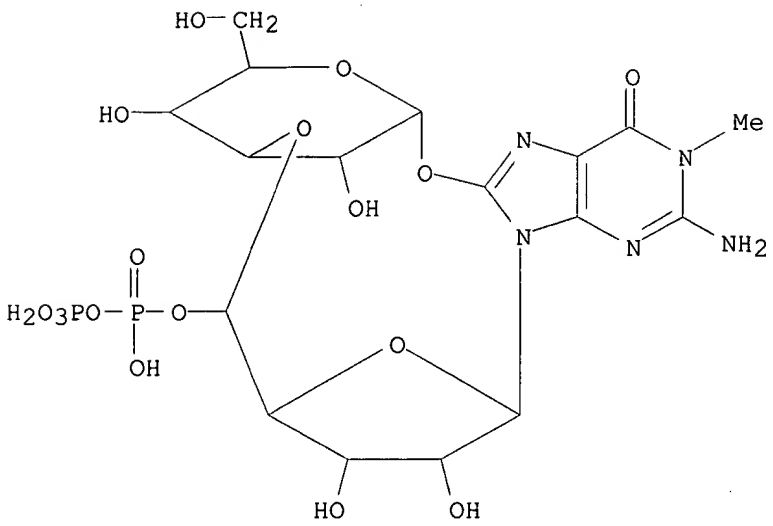
III R 1 = H, R2 = $CH_2OH$ $CO_2H$ $CH_2OH$ | | | $COCHNHCOCH_2CHNHCOCHNHCOCHNH_2$ | $CH_2OH$

AB Chitin synthase inhibitor guanofosfocin A (I) is manufd. with and isolated from Streptomyces sp., while guanofosfocins B and C (II and III, resp.) were isolated from Trichoderma sp. The structures of these chitin synthase inhibitors were detd. Also given are the IC50s of I-III against Candida albicans strains. They are considerably better than those of polyoxin D and nikkomycin Z.

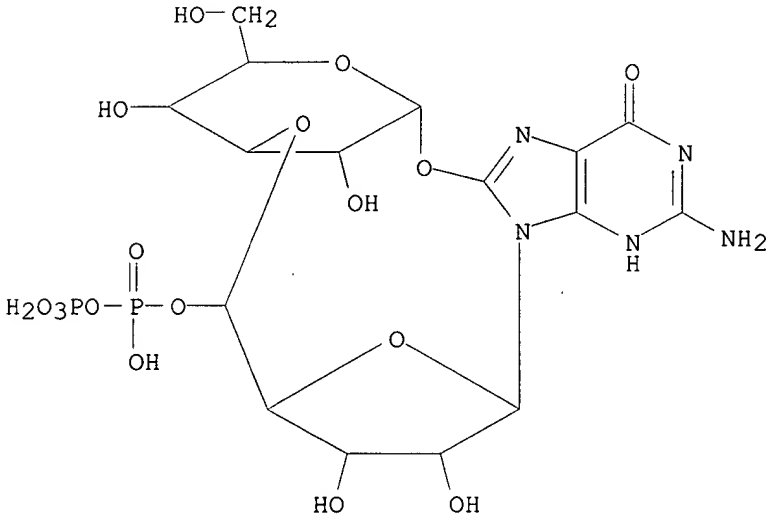
IT **183658-78-8P**, Guanofosfocin A **183658-79-9P**, Guanofosfocin B **183658-80-2P**, Guanofosfocin C
RL: BPN (Biosynthetic preparation); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(novel chitin synthase inhibitors; guanofosfocins produced by microorganism)

RN 183658-78-8 HCAPLUS

CN Diphosphoric acid, mono[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-2-amino-3,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-3-methyl-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-13-yl] ester (9CI) (CA INDEX NAME)

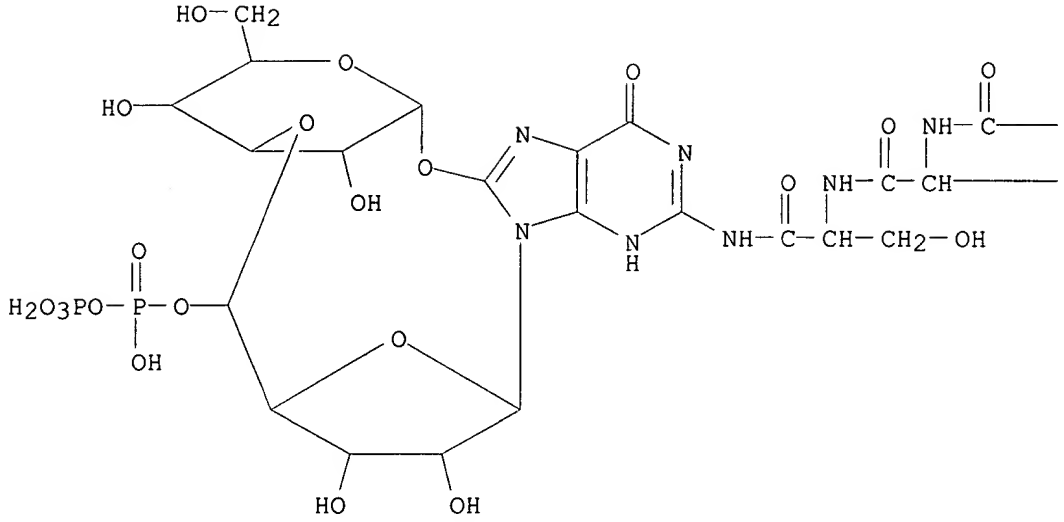


RN 183658-79-9 HCAPLUS
CN Diphosphoric acid, mono[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-2-amino-1,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-13-yl] ester (9CI) (CA INDEX NAME)

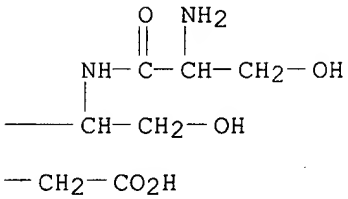


RN 183658-80-2 HCAPLUS
CN L-Serinamide, L-seryl-L-seryl-L-.alpha.-aspartyl-N-[(7R,9R,10R,11S,13S,14S,15S,16R,17R,20S)-1,4,10,11,14,15,16,17-octahydro-10,15,16,20-tetrahydroxy-9-(hydroxymethyl)-13-[[hydroxy(phosphonooxy)phosphinyl]oxy]-4-oxo-14,17-epoxy-7,11-methano-9H,13H-[1,3,11,5]trioxaazacyclotetradecino[5,4-e]purin-2-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L8 ANSWER 9 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:981828 HCAPLUS
DOCUMENT NUMBER: 124:111063
TITLE: Radiation chemistry of d(ApCpGpT)
AUTHOR(S): Schroder, E.; Budzinski, E. E.; Wallace, J. C.; Zimbrick, J. D.; Box, H. C.
CORPORATE SOURCE: Biophysics Dep., Roswell Park Center Inst., Buffalo, NY, 14263, USA
SOURCE: Int. J. Radiat. Biol. (1995), 68(5), 509-23
CODEN: IJRBE7; ISSN: 0955-3002
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The radiation chem. of the DNA tetranucleoside triphosphate d(ApCpGpT) was investigated. X-irradiations were carried out on aq. solns. satd. with oxygen (with and without added Cu++), nitrogen or nitrous oxide. When oxygen was present, the principal products were formed by hydroxylation at the 8-position of guanine and by degrdn. of thymine leaving a formamido remnant. Products were also formed contg. both of the aforementioned lesions at adjacent deoxyguanosine and pyrimidine nucleosides. Other products resulted from rearrangement of the thymine ring generating two diastereoisomers of the 5-methyl-5-hydroxyhydantoin modification of d(ApCpGpT). Rearrangement of the cytosine ring occurred generating

imidazolidine products and a hydantoin products. The product profiles are similar when either an N2O or N2 gaseous environment is maintained. However, in the latter case the dihydrothymine modifications of d(ApCpGpT) are markedly enhanced. Other products include an 8,5' cyclized product formed from the 2'-deoxyadenosine nucleoside and the 8-hydroxyguanine modification. 6-Hydroxy-5,6-dihydrothymine and 5,6-dihydroxy-5,6-dihydrothymine modifications of the thymidine nucleoside were also obsd. A strand break product formed in oxygenated soln. is also produced in nitrous oxide satd. solns. Scission of the deoxyadenosine terminus was also obsd. The effect of several of these lesions on d(ApCpGpT) as substrate for nuclease P1, bovine spleen phosphodiesterase and snake venom phosphodiesterase was studied.

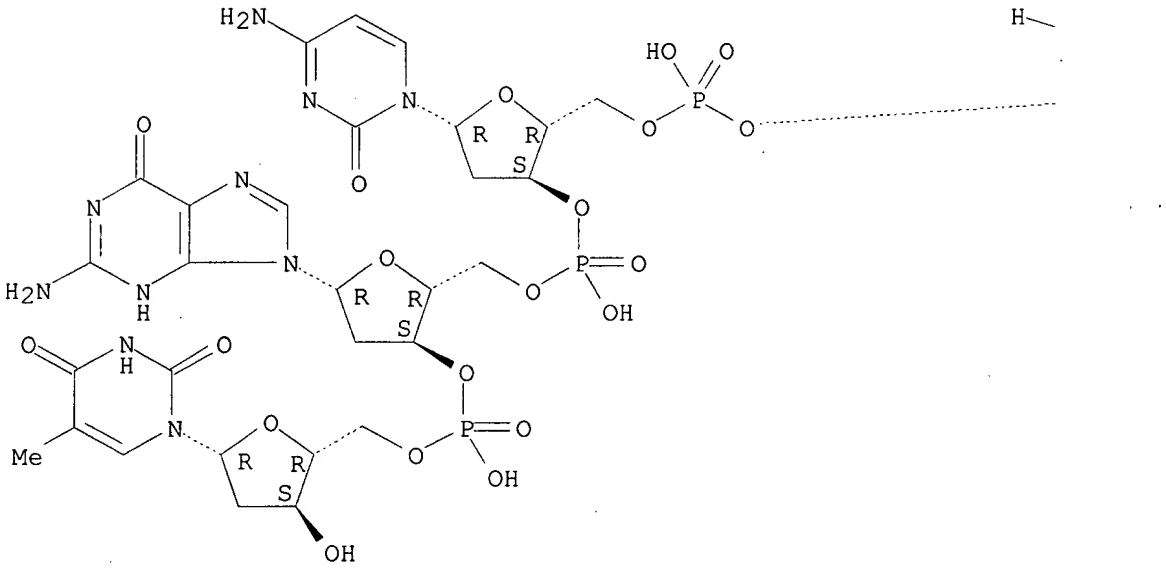
IT **172990-03-3**
RL: ANT (Analyte); FMU (Formation, unclassified); ANST (Analytical study); FORM (Formation, nonpreparative)
(radiation chem. of d(ApCpGpT))

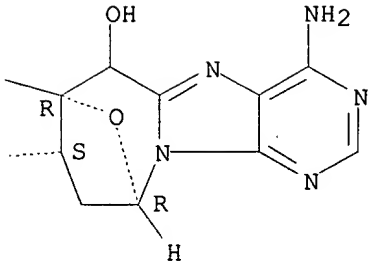
RN 172990-03-3 HCAPLUS

CN Thymidine, 2'-deoxy-5',8-C-cycloadenylyl-(3'.fwdarw.5')-2-deoxycytidylyl-(3'.fwdarw.5')-2-deoxyguanylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

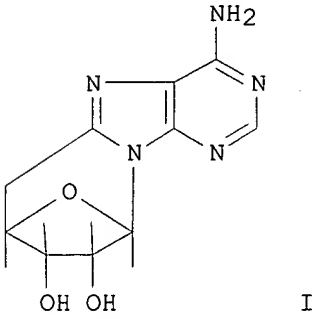
Absolute stereochemistry.

PAGE 1-A





L8 ANSWER 10 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:273414 HCAPLUS
DOCUMENT NUMBER: 122:240305
TITLE: Spectropolarimetric properties of some adenosine cyclic derivatives
AUTHOR(S): Morozov, Yu. V.; Bazhulina, N. P.; Bokovoy, V. A.; Savitskiy, A. V.; Chekhov, V. O.; Florentiev, V. L.
CORPORATE SOURCE: Engelhardt Inst. Mol. Biol., Russian Acad. Sci., Moscow, 117984, Russia
SOURCE: Mol. Biol. (Moscow) (1994), 28(6), 1330-40
CODEN: MOBIBO; ISSN: 0026-8984
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I

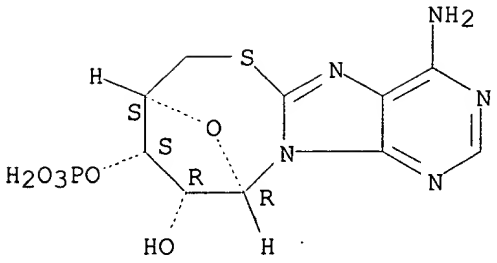
AB The CD spectra of tautomeric and protonated forms of adenosine cyclic derivs., e.g., I, are examd. Calcn. of the spectropolarimetric properties by methods such as CNDO/S are discussed.

IT **56828-07-0 68686-63-5 162240-50-8**
**162240-51-9**
RL: PRP (Properties)
(CD spectrum of)

RN 56828-07-0 HCAPLUS

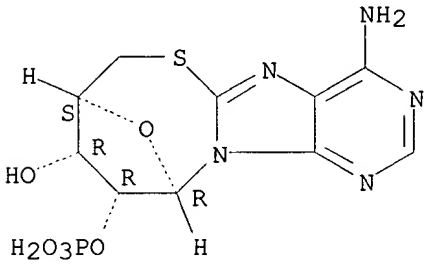
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 9-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



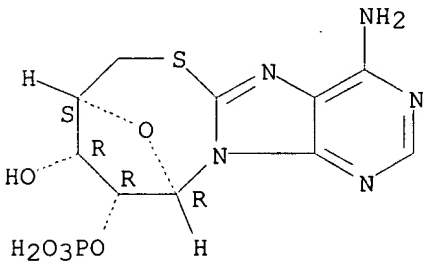
RN 68686-63-5 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 10-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



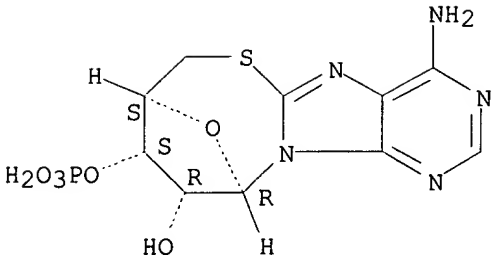
RN 162240-50-8 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 10-(dihydrogen phosphate), conjugate monoacid, [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 162240-51-9 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 9-(dihydrogen phosphate), conjugate monoacid, [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

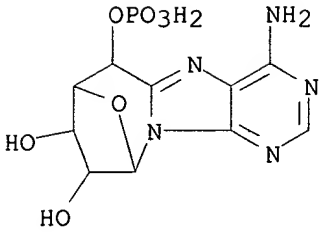
Absolute stereochemistry.



L8 ANSWER 11 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:64992 HCAPLUS
DOCUMENT NUMBER: 122:10443
TITLE: Irreversible Protonation Sites of One-Electron-Reduced Adenine: Comparisons between the C5 and the C2 or C8 Protonation Sites
AUTHOR(S): Barnes, Jeff; Bernhard, William A.
CORPORATE SOURCE: Department of Biophysics, University of Rochester, Rochester, NY, 14642, USA
SOURCE: J. Phys. Chem. (1994), 98(42), 10969-77
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reversible and irreversible protonation sites of one-electron-reduced adenine are shown to depend upon the environment adenine is reduced in. Redn. of 2'-deoxyadenosine in a PEG glass (polyethylene glycol, 12 M monomer) at 77 K probably gives rise to the neutral, N1-protonated reduced adenine radical. Upon annealing to .apprx.150 K, an irreversible protonation at C2 or C8 is obsd. Upon redn. at 4 K in a high-salt glass contg. Li+ or Mg2+, 5'AMP protonates at the amino group, which assumes an sp3 conformation with one N-H bond perpendicular to the ring plane. A second, irreversible protonation occurs at C5 upon annealing to 40-80 K. This adenine radical is identified by a distinctive set of EPR and optical absorption spectra. The reaction pathway leading to protonation at C5 could be a significant trap for mobile electrons in X-irradiated, single-stranded DNA.

IT **41036-59-3**
RL: RCT (Reactant)
(irreversible protonation sites of one-electron-reduced adenine of DNA and comparisons between the C5 and the C2 or C8 protonation sites)
RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)

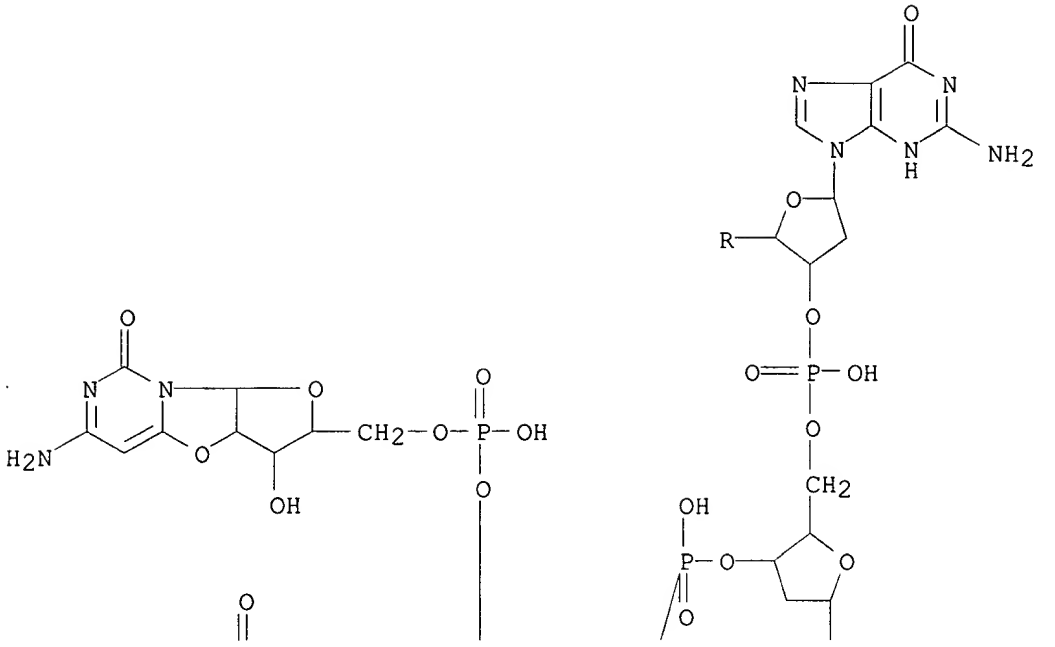



L8 ANSWER 12 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:624419 HCAPLUS
DOCUMENT NUMBER: 121:224419
TITLE: Monoclonal antibodies with affinity to self-complementary left-handed DNA containing cyclonucleosides with high anti conformation
AUTHOR(S): Kawakami, Junji; Uesugi, Seiichi; Ikehara, Morio; Itoh, Teiji; Miura, Kazunobu; Ohtsuka, Eiko
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan
SOURCE: Nucleosides Nucleotides (1994), 13(1-3), 421-7
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Monoclonal antibodies specific for a self-complementary hexanucleotide with a high-anti conformation were found to bind another hexanucleotide with a high-anti conformation, but with a different sequence. A higher order structure seemed to be recognized in the reaction.

IT **109081-57-4**
RL: PRP (Properties)
(double-stranded, prepn.)
RN 109081-57-4 HCAPLUS
CN .beta.-D-arabino-Cytidine, 2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2'-deoxycytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



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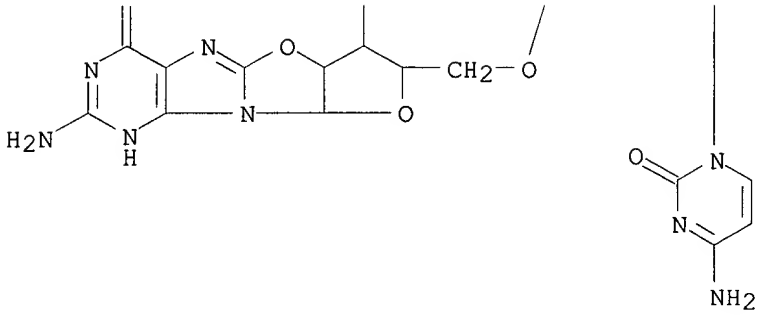
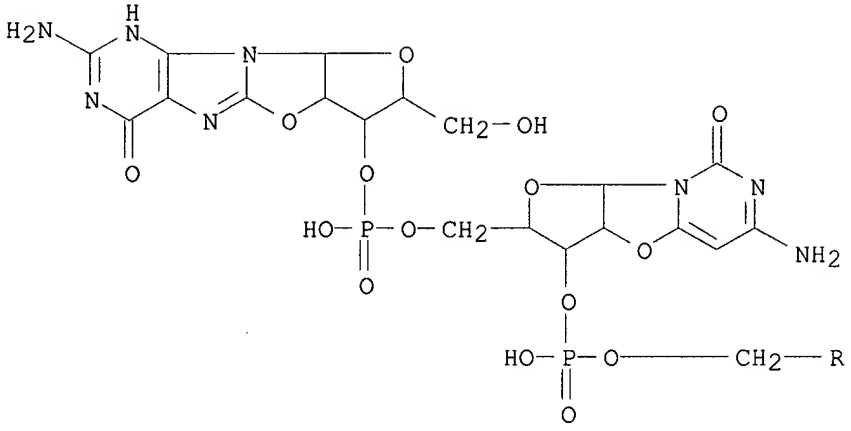
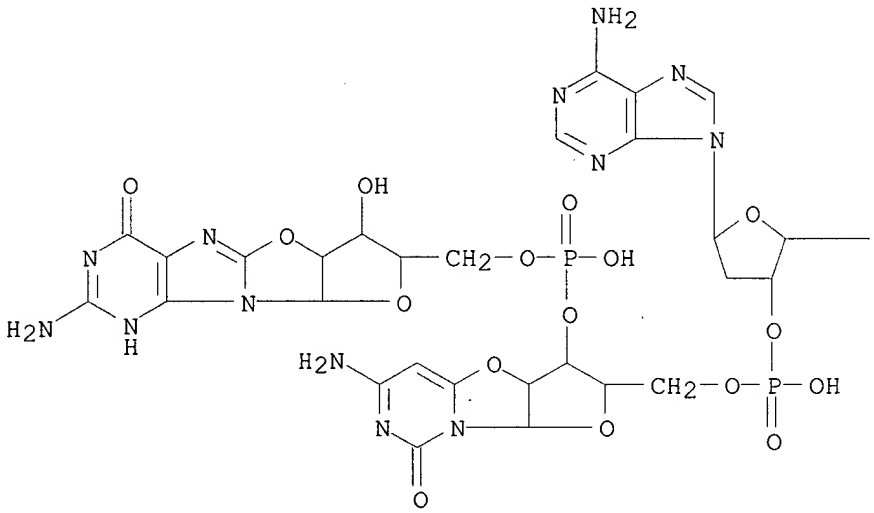


PAGE 3-A

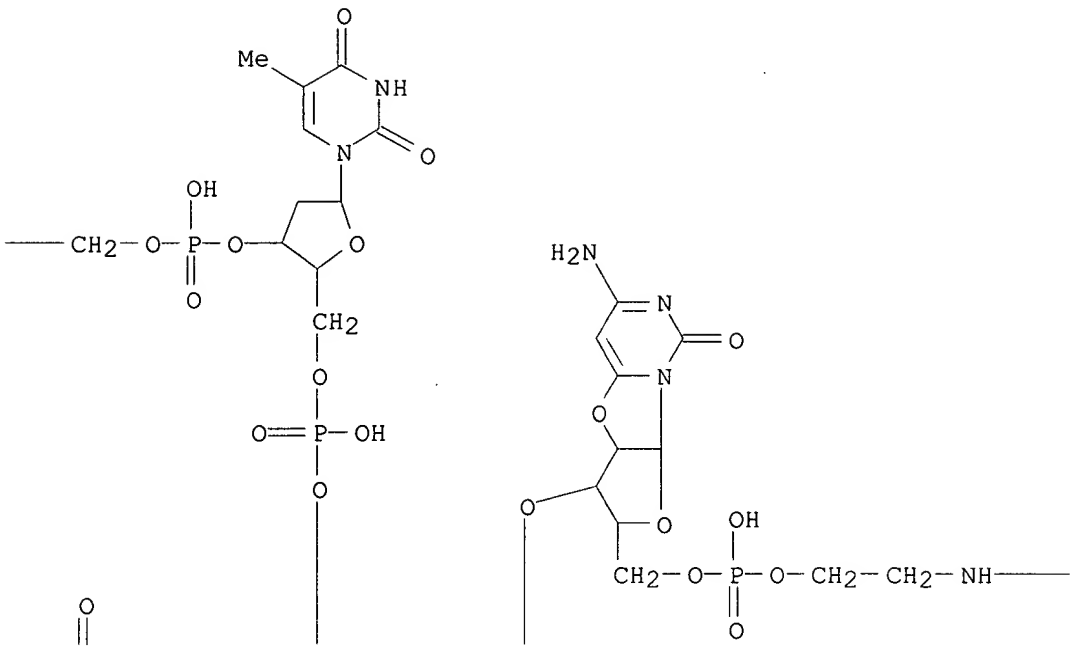


IT **158080-77-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(double-stranded, prepn. and monoclonal antibodies recognition on high-anti conformation of)
RN 158080-77-4 HCAPLUS
CN .beta.-D-arabino-Guanosine, 2',6-anhydro-5'-O-[[2-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]ethoxy]hydroxyphosphinyl]-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

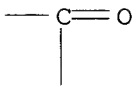
PAGE 1-A



PAGE 1-B



PAGE 1-C



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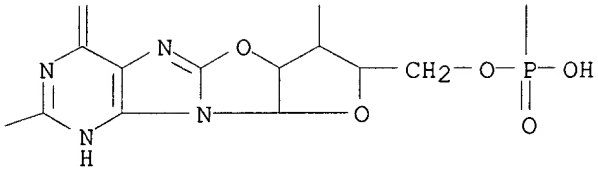
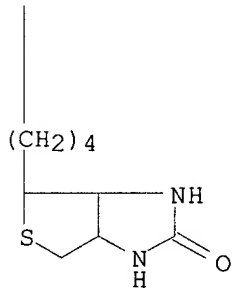
PAGE 2-B

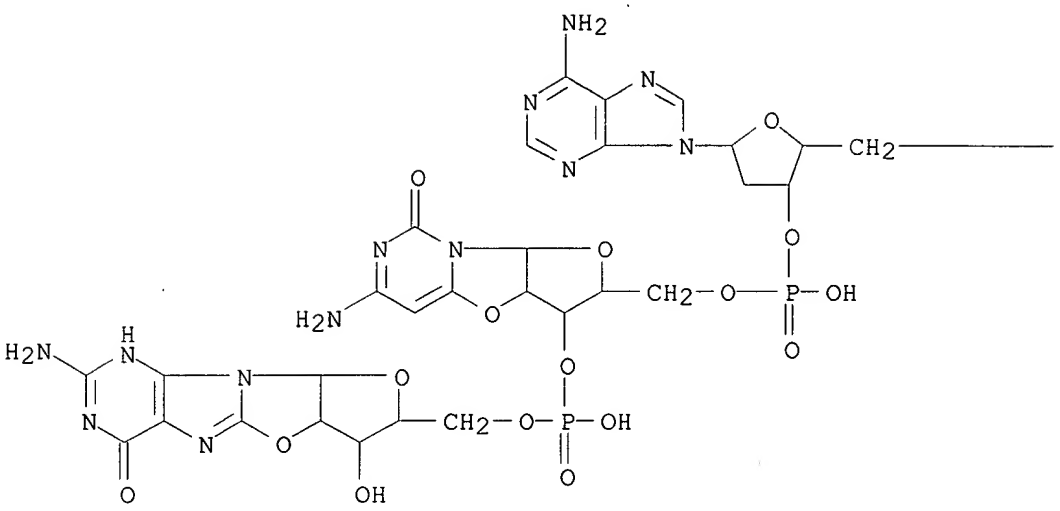


PAGE 2-C

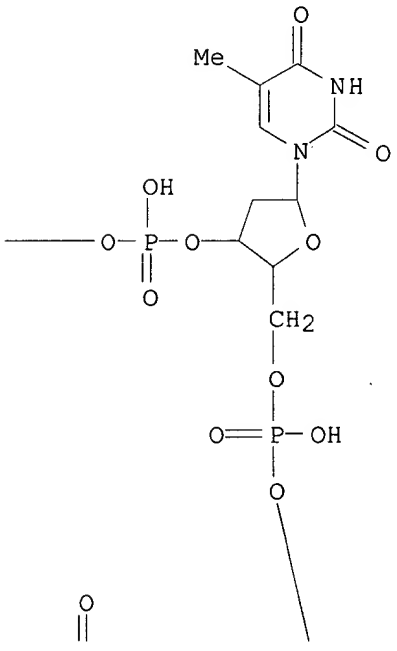


IT **158080-85-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and biotinylation of)
RN 158080-85-4 HCAPLUS
CN .beta.-D-arabino-Guanosine, 5'-O-[(2-aminoethoxy)hydroxyphosphinyl]-2',8-anhydro-8-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



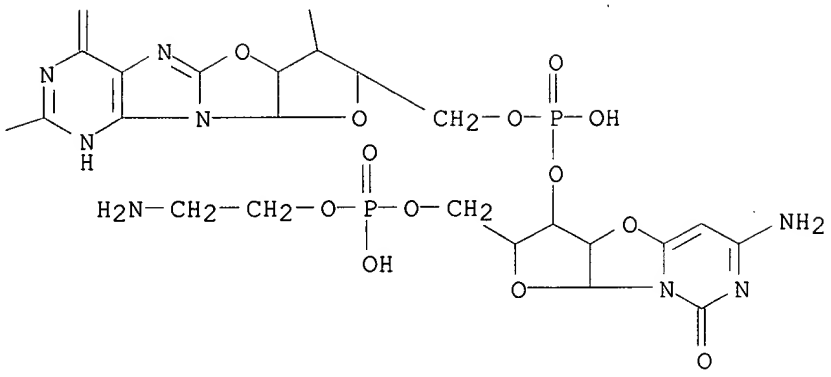
PAGE 1-B



PAGE 2-A

$H_2N$

PAGE 2-B



L8 ANSWER 13 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:157850 HCAPLUS
DOCUMENT NUMBER: 120:157850
TITLE: An evaluation of proton spin-lattice relaxation rates and NOE's for calibration of interproton distance measurements in nucleic acids
AUTHOR(S): Kan, Lou Sing; Boal, Jila; Ts'o, Paul O. P.
CORPORATE SOURCE: Inst. Chem., Acad. Sin., Taipei, 115, Taiwan
SOURCE: Bull. Inst. Chem., Acad. Sin. (1993), 40 55-66
CODEN: BICMAD; ISSN: 0366-0370
DOCUMENT TYPE: Journal
LANGUAGE: English

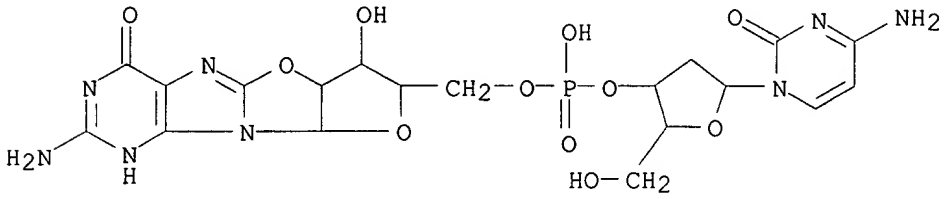
AB A combination of 1H spin-lattice relaxation rates (1/T1) and 1H-1H NOE studies were performed on 2'-deoxycytidine 5'-monophosphate (dCMP), 2'-deoxycytidyl(3'-5')8,2'-anhydro-1-.beta.-D-arabinofurosyl-8-hydroxyguanosine (CpG.degree.), and 8,2'-anhydro-1-.beta.-D-arabinofurosyl-8-hydroxyguanylyl (3'-5') 2'-deoxycytidine (G.degree.pC) for quant. evaluation of the proton-proton distance detn. by NMR spectroscopy. This is because both nucleotidyl moieties in the dimer as well as the monomeric dCMP harbor at least one pair protons in adjacent carbon atoms with fixed conformation. Thus, the interproton distances are also fixed. The distance between H5 and H6 in dCMP detd. by T1 measurement is very closed to that derived from the X-ray diffraction data. Similar results were obsd. in the distances of H5-H6 and H1'-H2" in those two dimers by T1 measurement. The NOE results are compliant to that from T1 measurements in the case of adjacent protons. The errors increased in the longer distances (H1'-H6). The reliability of the detn. of interproton distances by comparison of NOE with a ref. distance is discussed.

IT **153311-50-3 153311-51-4**
RL: ANST (Analytical study)
(proton spin-lattice relaxation rates and NOEs for interproton distance

measurement in nucleic acids in relation to)

RN 153311-50-3 HCAPLUS

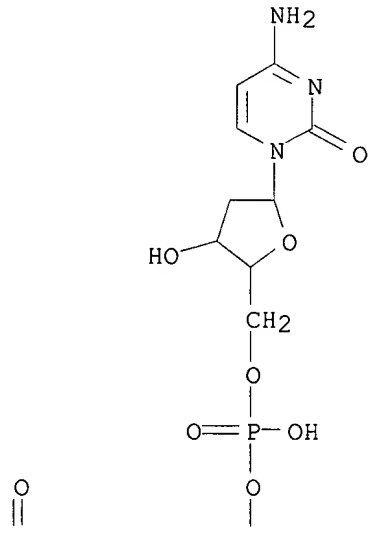
CN Guanosine, 2'-deoxycytidylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epoxy- (9CI) (CA INDEX NAME)



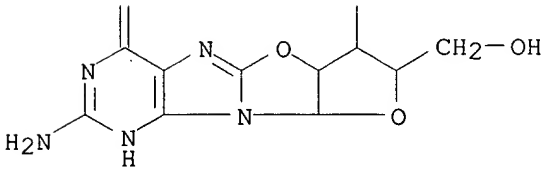
RN 153311-51-4 HCAPLUS

CN Cytidine, 2'-deoxy-2',8-epoxyguanylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

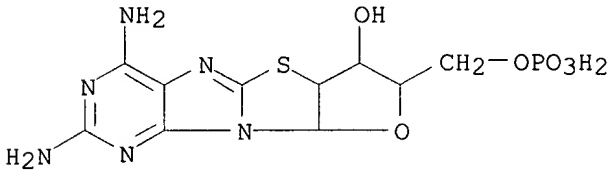


L8 ANSWER 14 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:631892 HCAPLUS
DOCUMENT NUMBER: 113:231892
TITLE: Synthesis and properties of dinucleoside monophosphates containing 2-aminoadenine 8,2'-S- and uracil 6,2'-O-cyclonucleosides
AUTHOR(S): Muraoka, Masako; Takahashi, Seizo; Yamaguchi, Naoko; Oda, Yasushi; Uesugi, Seiichi
CORPORATE SOURCE: Dep. Chem., Japan Women's Univ., Tokyo, 112, Japan
SOURCE: Nucleosides Nucleotides (1990), 9(2), 205-21
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:231892
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

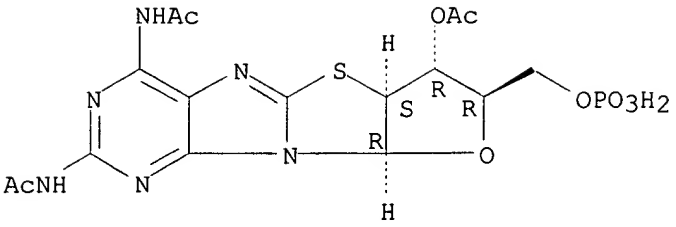
AB Two sequence isomers of dinucleoside monophosphates contg. 8,2'-anhydro-2,6-diamino-8-mercapto-9-.beta.-D-arabinofuranosylpurine (2NH2As) and 6,2-anhydro-6-hydroxy-1-.beta.-D-arabinofuranosyluracil (Uo), 2NH2AspUo (I) and Uop2NH2As(II) were synthesized by the phosphodiester method. Examn. of the UV, CD and NMR spectra of these dimers led us to the conclusion that, whereas I did not take a stacked conformation, II took a well stacked conformation in which the bases were stacked along a left-handed screw axis. Both the dimers formed a complex with ethidium bromide.

IT **130471-91-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 130471-91-9 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 2,4-diamino-6a,7,8,9a-tetrahydro-7-hydroxy-, 8-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

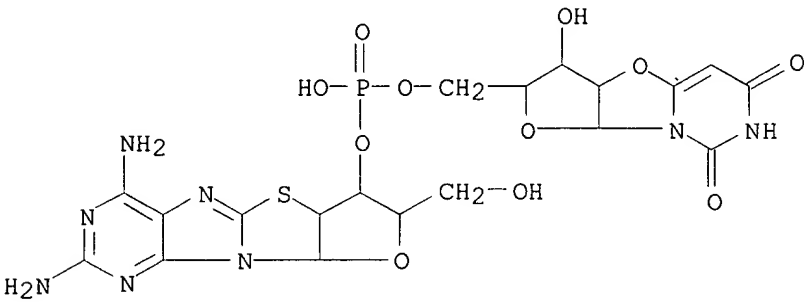



IT **130471-90-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling of, with uracil cyclonucleoside)
RN 130471-90-8 HCAPLUS
CN Acetamide, N,N'-[7-(acetyloxy)-6a,7,8,9a-tetrahydro-8-[(phosphonooxy)methyl]furo[2',3':4,5]thiazolo[3,2-e]purine-2,4-diyl]bis-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

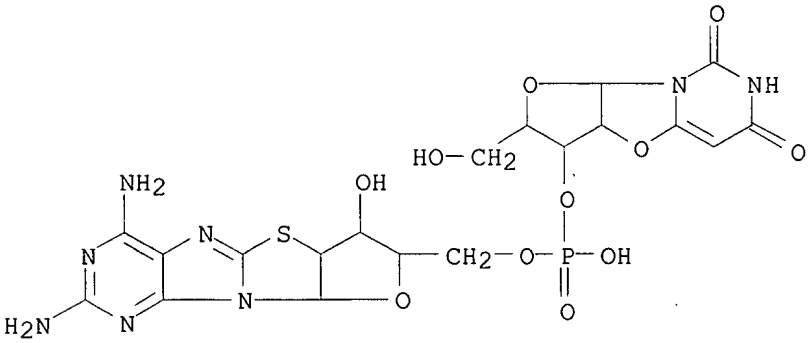
Absolute stereochemistry.



IT **130446-14-9P 130446-15-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and stacking conformation of)
RN 130446-14-9 HCAPLUS
CN .beta.-D-arabino-Uridine, 2-amino-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',6-epoxy- (9CI) (CA INDEX NAME)

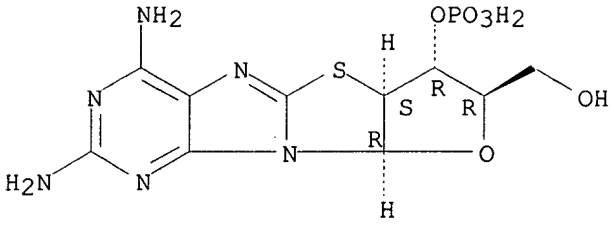


RN 130446-15-0 HCAPLUS
CN Araadenosine, 2'-deoxy-2',6-epoxyarauridylyl-(3'.fwdarw.5')-2-amino-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



IT **130471-92-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 130471-92-0 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 2,4-diamino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

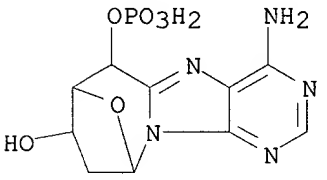


L8 ANSWER 15 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:213121 HCAPLUS
DOCUMENT NUMBER: 112:213121
TITLE: Formation of .alpha.-deoxyadenosine in polydeoxynucleotides exposed to ionizing radiation under anoxic conditions
AUTHOR(S): Lesiak, Krystyna B.; Wheeler, Kenneth T.
CORPORATE SOURCE: Med. Cent., Wake Forest Univ., Winston-Salem, NC, 27103, USA
SOURCE: Radiat. Res. (1990), 121(3), 328-37
CODEN: RAREAE; ISSN: 0033-7587
DOCUMENT TYPE: Journal
LANGUAGE: English

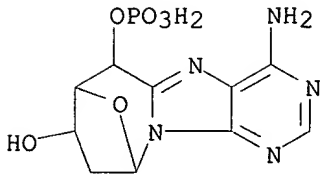
AB When poly(dA), poly(dA-dT), and salmon testis DNA were .gamma.-irradiated under N, the major deoxyadenosine damage product (excluding liberated adenine) was identified as the .alpha.-anomer of deoxyadenosine. The yields of .alpha.-deoxyadenosine from poly(dA), poly(dA-dT), and salmon testis DNA irradiated with a dose of 500 Gy under anoxic conditions were 1.5, 1.3, and 1.3%, resp. No .alpha.-deoxyadenosine was detected after irradn. under oxic conditions. The presence of nucleotides with the .alpha.-configuration at the anomeric C atom in the DNA chain may have a significant effect on its tertiary structure and possibly modify its biol. activity.

IT **126847-37-8 126847-38-9**
RL: FORM (Formation, nonpreparative)
(formation of, in polydeoxynucleotides after gamma-irradn. under anoxic conditions)

RN 126847-37-8 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8-diol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)



RN 126847-38-9 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8-diol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,10.beta.)]- (9CI) (CA INDEX NAME)

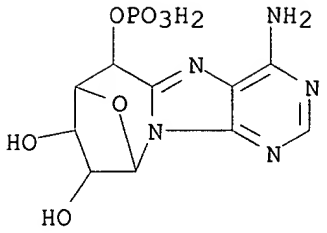



L8 ANSWER 16 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:194412 HCAPLUS
DOCUMENT NUMBER: 112:194412
TITLE: Structural requirements for the binding of AMP to the allosteric site of NAD-specific isocitrate dehydrogenase from bakers' yeast
AUTHOR(S): Gabriel, Jerome L.; Plaut, Gerhard W. E.
CORPORATE SOURCE: Sch. Med., Temple Univ., Philadelphia, PA, 19140, USA
SOURCE: Biochemistry (1990), 29(14), 3528-35
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

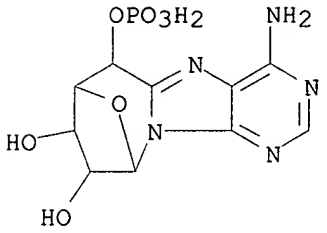
AB The specificity of yeast NAD-specific isocitrate dehydrogenase for the structures of the allosteric effector, AMP, was examd. with analogs modified in the purine ring, pentosyl group, and 5'-phosphate group. An unsubstituted 6-amino group was essential for activation as was the phosphoryl group at the 5'-position. Activity was retained when an O function of the 5'-phosphoryl was replaced by S or by N (phosphoramidates). 2-NH2-AMP, 2-azido-AMP, and 8-NH2-AMP were active; 8-azido-AMP and 8-Br-AMP were inactive. The configuration or nature of substituents about C-2' and C-3' of the pentosyl portion of AMP was not crit. for allosteric activation since AMP analogs contg., e.g., 2',3'-dideoxyribose or the bulky 2',3'-O-(2,4,6-trinitrocyclohexadienylidene) substituent (TNP-AMP) were active. TNP-AMP was bound to the enzyme with fluorescence enhancement and had an S0.5 for activation similar to the S0.5 for AMP. Pos. effector activity was decreased when the pentosyl moiety of AMP was replaced by the 6-membered N-contg. morpholine group, indicating that the pentosyl group may be crit. as a spacer for the proper geometry of binding to enzyme at the 6-amino and 5'-phosphoryl groups of AMP. A comparison of mol. models of AMP with 8,5'-cycloAMP suggested that the species of AMP required for binding to the enzyme contains the purine and ribose moieties in an anti conformation and positioning of the 5'-phosphate trans with respect to C-4'. This was consistent with the finding that (S)-8,5'-cycloAMP was a potent neg. allosteric modifier (i.e., it increased the Km for isocitrate) whose effect could be reversed competitively by AMP, whereas the R epimer was inactive.

IT **41036-59-3 41116-92-1**
RL: BIOL (Biological study)
(isocitrate dehydrogenase of yeast response to, structure in relation to)

RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)

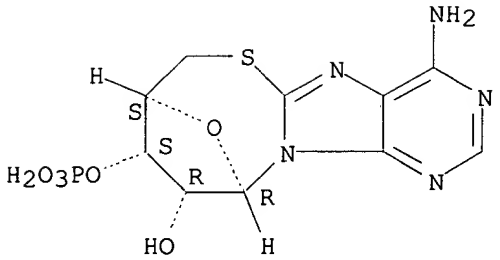


RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)



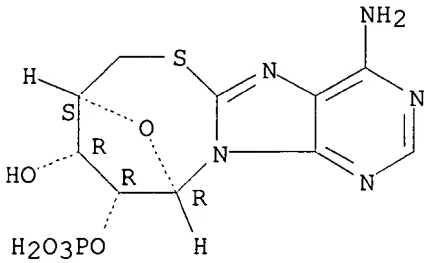
L8 ANSWER 17 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1990:134637 HCAPLUS
DOCUMENT NUMBER: 112:134637
TITLE: Acyclonucleosides. Electronic structure and spectral properties
AUTHOR(S): Morozov, Yu. V.; Bokovoi, V. A.; Bazhulina, N. P.; Chekhov, V. O.; Florent'ev, V. L.
CORPORATE SOURCE: V. A. Engel'hardt Inst. Mol. Biol., Moscow, 117984, USSR
SOURCE: Mol. Biol. (Moscow) (1989), 23(6), 1658-68
CODEN: MOBIBO; ISSN: 0026-8984
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Electronic structure, spectral properties, and acid-based and tautomeric equil. of some adenosine acyclo derivs. were investigated. A characteristic of the compds. under investigation is their conformational rigidness. Unlike adenosine, some of the compds. exist in soln. in amino- and imino-forms whose interrelations were derived from spectroscopic data. Electronic structure of the amino-tautomers is identical to that of corresponding ionic forms of adenine, whereas the structure of imino-tautomers is identical to that of analogous forms of hypoxanthine.
IT **56828-07-0 68686-63-5**
RL: BIOL (Biological study)
(electronic structure and spectral properties of)
RN 56828-07-0 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 9-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 68686-63-5 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 10-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



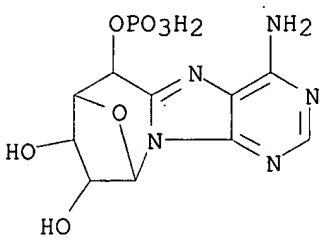
L8 ANSWER 18 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:164097 HCAPLUS
DOCUMENT NUMBER: 108:164097
TITLE: Oxygen dependence of product formation in irradiated adenosine 5'-monophosphate
AUTHOR(S): Fuciarelli, A. F.; Koch, C. J.; Raleigh, J. A.
CORPORATE SOURCE: Cross Cancer Inst., Edmonton, AB, T6G 1Z2, Can.
SOURCE: Radiat. Res. (1988), 113(3), 447-57
CODEN: RAREAE; ISSN: 0033-7587
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The formation of (R)- and (S)-8,5'-cycloadenosine-5'-monophosphate (8,5'-cycloAMP), 8-hydroxyadenosine 5'-monophosphate (8-hydroxyAMP), and radiolytic adenine release from irradiated solns. of 5'-AMP was measured as a function of increasing liq.-phase O concn. Three classes of specific mol. damage were identified on the basis of the O dependence for product formation. Major changes in product yield occurred near the range of O concns. assocd. with the radiobiol. O effect. In addn. to these data, systematic increases in the concn. of H2O2 at the time of irradn. resulted in an increase in the yield of 8-hydroxyAMP and a component of radiolytic adenine release in N-satd. solns. of 5'-AMP. However, no changes in the yield of the 8,5'-cyclonucleotides were obsd. under these conditions.

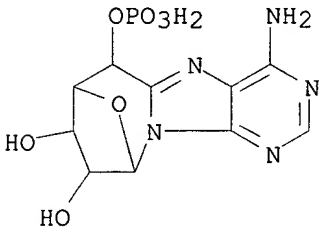
IT **41036-59-3**, (S)-8,5'-Cycloadenosine 5'-monophosphate (8,5'-cycloAMP) **41116-92-1**, (R)-8,5'-Cycloadenosine-5'-monophosphate
RL: FORM (Formation, nonpreparative)
(formation of, from AMP radiolysis in aq. soln., oxygen dependence of)

RN 41036-59-3 HCAPLUS

CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)




RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)




L8 ANSWER 19 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:51447 HCAPLUS
DOCUMENT NUMBER: 108:51447
TITLE: Hybrid hexanucleotide duplex containing cyclonucleotides and deoxynucleotides: the d(TA) segment can adopt a high anti left-handed double-helical structure
AUTHOR(S): Uesugi, Seiichi; Lee, Bok Luel; Ikehara, Morio; Fujii, Satoshi; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan
SOURCE: Biochemistry (1988), 27(2), 521-5
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In order to see whether DNA which contains cyclonucleotides can adopt a high anti left-handed double-helical structure, a self-complementary hexanucleotide contg. 6,2'-O-cyclocytidine (Co), 8,2'-O-cycloguanosine (Go), thymidine, and deoxyadenosine, CoGodTdACoGo, was synthesized. Imino proton NMR spectra and the results of NOE expts. strongly suggest that CoGodTdACoGo adopts a left-handed double-helical structure where the deoxynucleoside residues are involved in H bonding and take a high anti glycosidic conformation. A conformational model of the left-handed duplex was obtained by calcn. with energy minimization. Thus, it appears that DNA can form a high anti, left-handed double helix under some constrained conditions which is quite different from that of Z-DNA.

IT **112220-27-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(double-stranded, prepn. and high-anti left-handed conformation of, as

DNA model)

RN 112220-27-6 HCAPLUS

CN .beta.-D-arabino-Guanosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-2-deoxyadenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

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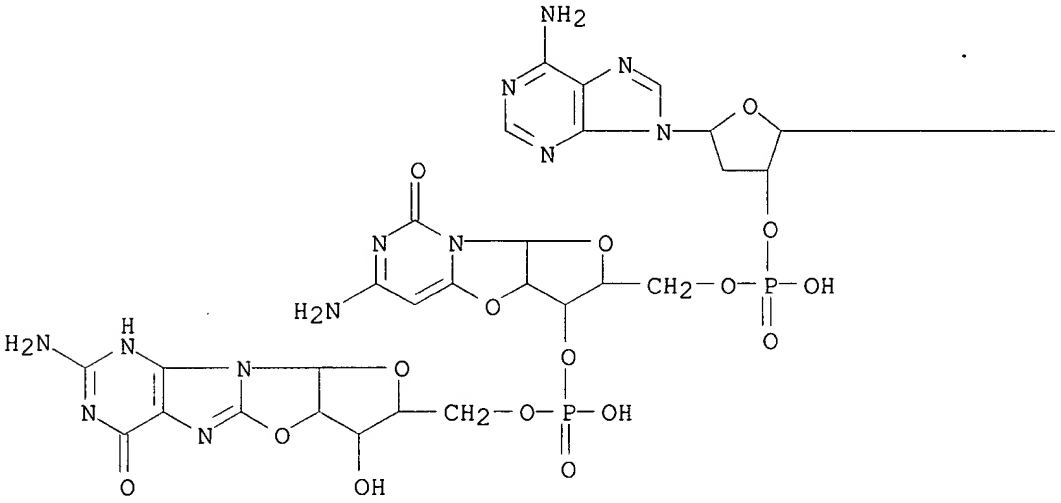
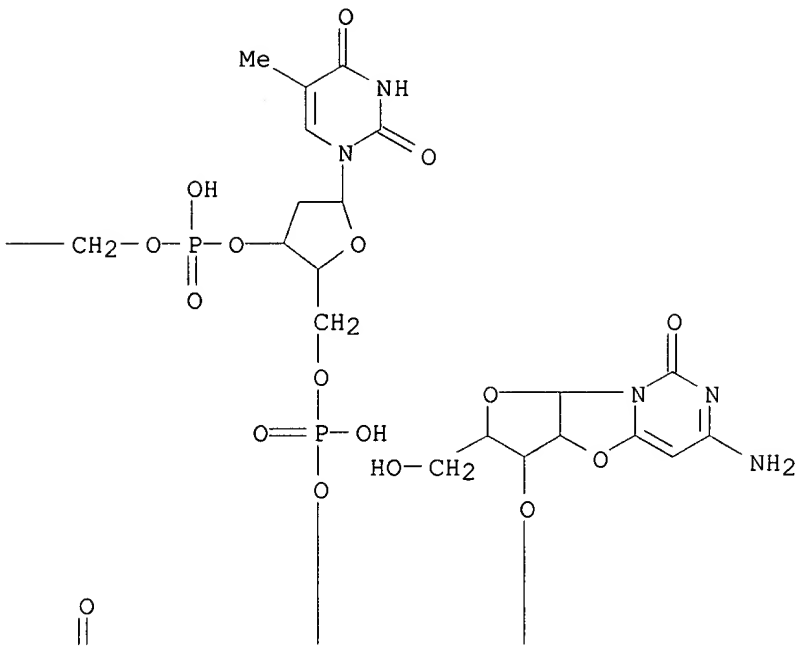


PAGE 1-B



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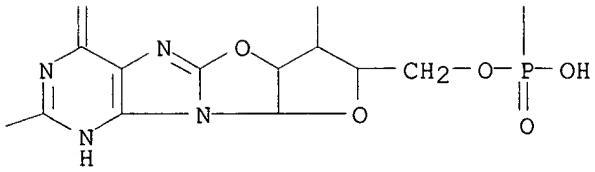
PAGE 2-B



L8 ANSWER 20 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:437733 HCAPLUS
DOCUMENT NUMBER: 107:37733
TITLE: Preparation and characterization of monoclonal antibodies specific for GOCOdGdCGOCO duplex with high-anti conformation
AUTHOR(S): Miura, Kazunobu; Saito, Miho; Itoh, Teiji; Ohtsuka, Eiko; Uesugi, Seiichi; Lee, Bok Luel; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan

SOURCE: Biochem. Biophys. Res. Commun. (1987), 144(2), 930-5
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

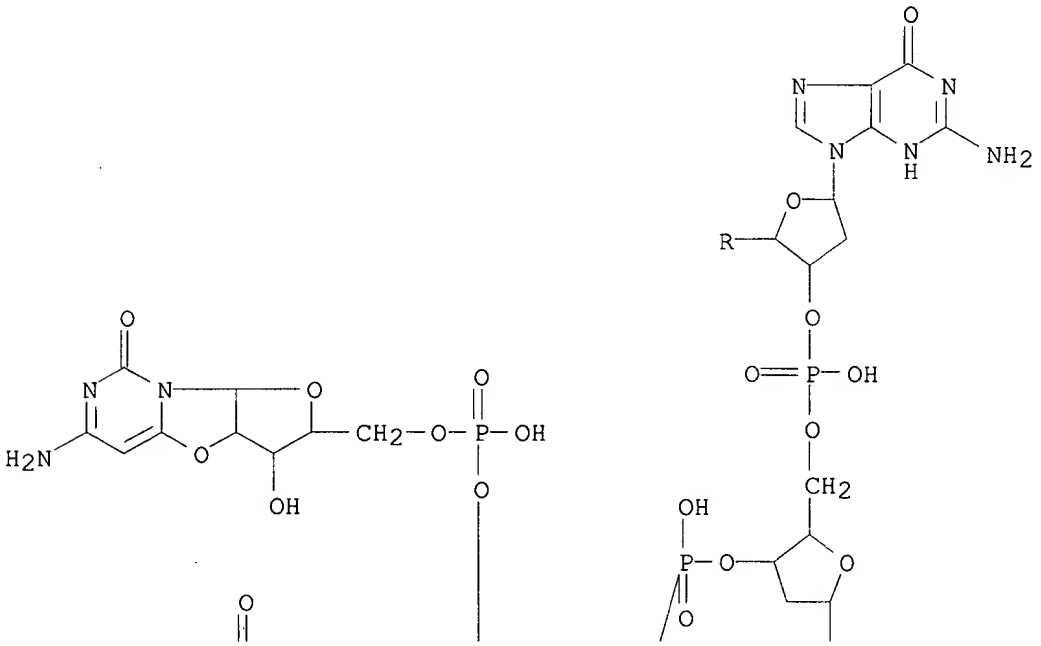
AB Monoclonal antibodies were prepd. using a self-complementary oligonucleotide duplex contg. cyclonucleosides with the high-anti conformation as an antigen. A competition ELISA assay showed that the monoclonal antibodies specifically recognized high-anti left-handed oligonucleotides but not oligonucleotides with B- or Z-conformation.

IT **109081-57-4P**
RL: PREP (Preparation)
(double-stranded, monoclonal antibodies specific for, prepn. and characterization of)

RN 109081-57-4 HCAPLUS

CN .beta.-D-arabino-Cytidine, 2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2'-deoxycytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



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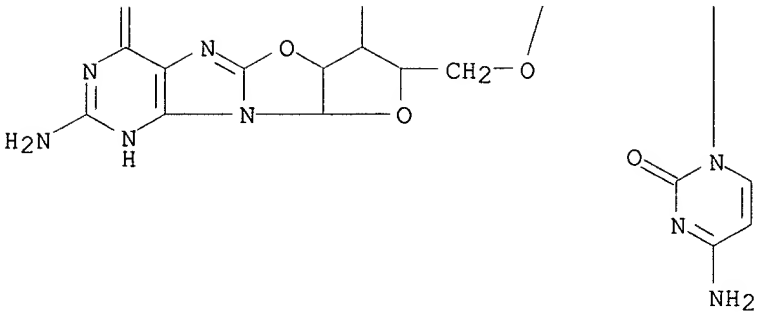
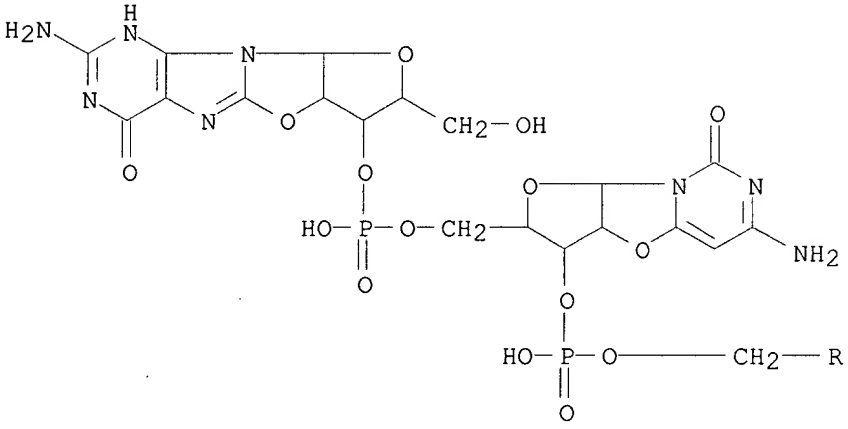


PAGE 3-A



IT **99499-17-9**
RL: BIOL (Biological study)
(monoclonal antibodies to high-anti left-handed oligonucleotide duplex binding to)
RN 99499-17-9 HCAPLUS
CN .beta.-D-arabino-Guanosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2'-deoxycytidylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

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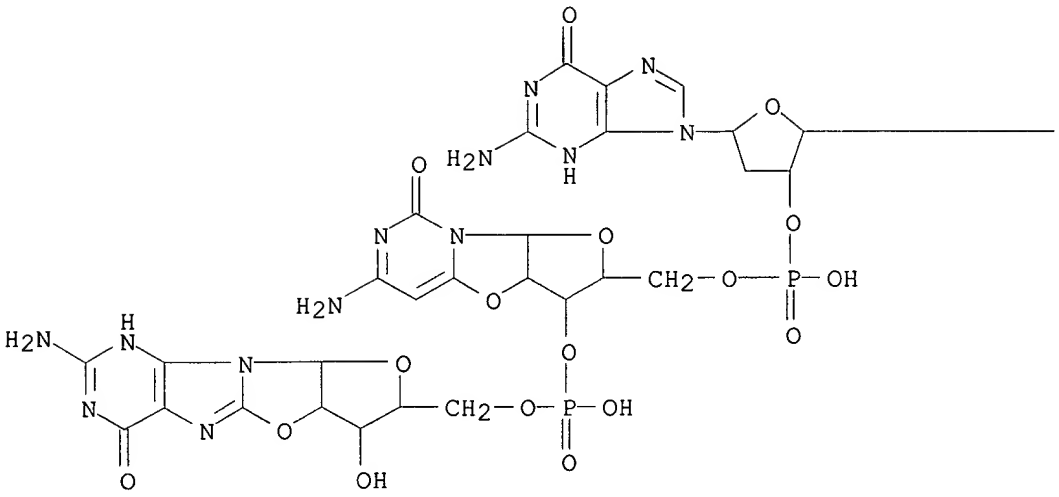
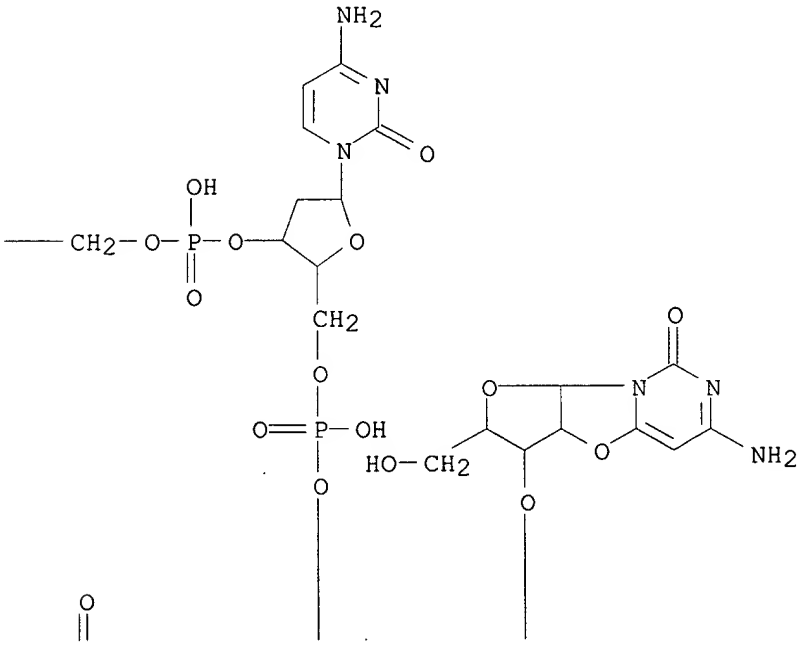


PAGE 1-B



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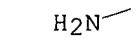

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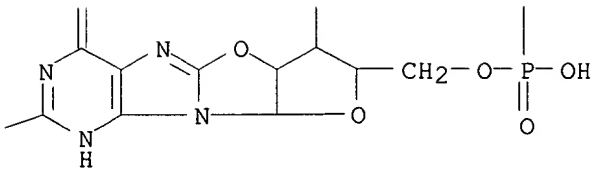

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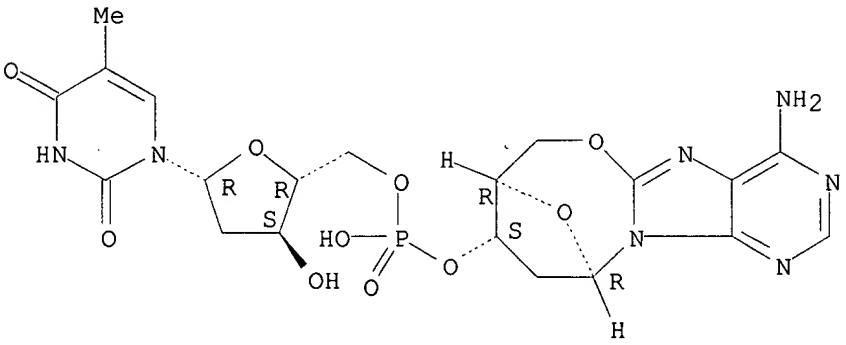
L8 ANSWER 21 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:172000 HCAPLUS
DOCUMENT NUMBER: 106:172000
TITLE: Radiation damage to dinucleoside monophosphates: mediated versus direct damage
AUTHOR(S): Paul, Chitta R.; Belfi, Charles A.; Arakali, Aruna V.; Box, Harold C.
CORPORATE SOURCE: Biophys. Dep., Roswell Park Mem. Inst., Buffalo, NY, 14263, USA
SOURCE: Int. J. Radiat. Biol. Relat. Stud. Phys., Chem. Med. (1987), 51(1), 103-14
CODEN: IJRBA3; ISSN: 0020-7616
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mediation of radiation-induced damage to dinucleoside monophosphate by O and by glutathione was studied. The sequence isomers d(TpA) and d(ApT) were x-irradiated in aq. solns. and the products isolated by reversed-phase HPLC. The main products were characterized by proton NMR spectroscopy. In the presence of O, the principal products are the formamido deriv. formed by breakdown of thymine and the aldehyde deriv. formed at the 5' end of the dinucleoside monophosphate, both nucleoside monophosphates and free bases. In the presence of glutathione, the 2 stereoisomers of the 5,6-dihydrothymine derivs. are prominent. Radiation-induced damage to d(TpA) and d(ApT) in the solid state was also studied.
IT **107856-87-1**
RL: FORM (Formation, nonpreparative)
(formation of, from dinucleoside monophosphates after radiolysis)
RN 107856-87-1 HCAPLUS
CN Thymidine, 5',8-anhydro-2'-deoxy-8-hydroxyadenylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




L8 ANSWER 22 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1987:80525 HCAPLUS
DOCUMENT NUMBER: 106:80525
TITLE: The molecular structure of cyclonucleotide hexamer, CoGoCoGoCoGo having a high-anti conformation
AUTHOR(S): Aragishi, Atsushi; Fujii, Satoshi; Uesugi, Seiichi; Lee, Bok Luel; Ikehara, Morio; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, 565, Japan
SOURCE: Nucleic Acids Symp. Ser. (1986), 17(Symp. Nucleic

Acids Chem., 14th, 1986), 227-30
CODEN: NACSD8; ISSN: 0261-3166
DOCUMENT TYPE: Journal
LANGUAGE: English

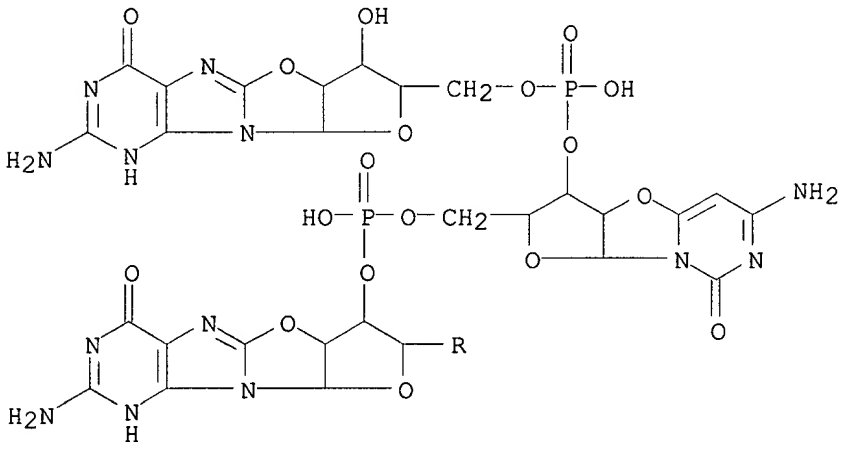
AB A cyclonucleotide hexamer, C0G0C0G0C0G0, was synthesized and crystd. as orthorhombic crystals with space group C2221, and unit cell dimensions a = 48.30, b = 41.53, and c = 31.76 .ANG.. The x-ray diffraction data up to 1.8-.ANG. resoln. were collected, and the crystal structure anal. by mol. replacement technique is now in progress using 2 energetically adequate left-handed helical models, obtained by conformational energy calcn.

IT **99486-53-0**
RL: BIOL (Biological study)
(double-stranded, crystn. and crystal structure of)

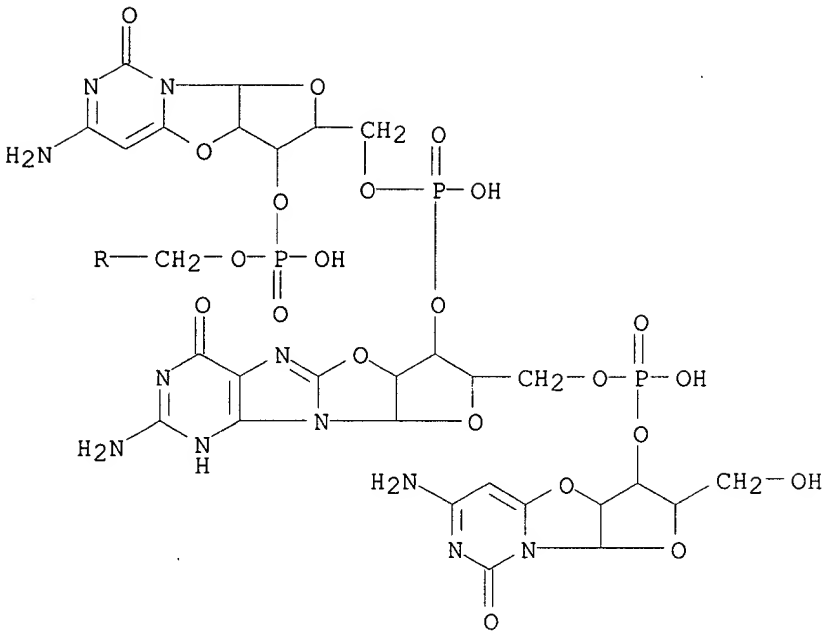
RN 99486-53-0 HCAPLUS

CN .beta.-D-arabino-Guanosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

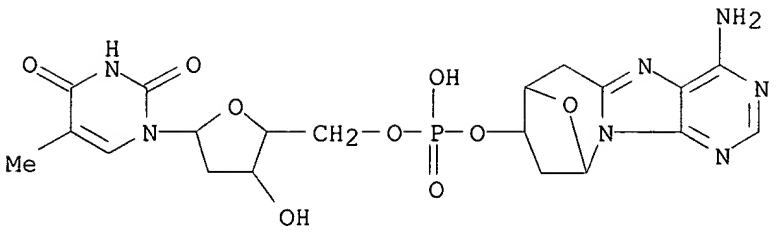


L8 ANSWER 23 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:438248 HCAPLUS
DOCUMENT NUMBER: 105:38248
TITLE: Radiation chemistry of a dinucleoside monophosphate and its sequence isomer
AUTHOR(S): Belfi, Charles A.; Arakali, Aruna V.; Paul, Chitta R.; Box, Harold C.
CORPORATE SOURCE: Biophys. Dep., Roswell Park Mem. Inst., Buffalo, NY, 14623, USA
SOURCE: Radiat. Res. (1986), 106(1), 17-30
CODEN: RAREAE; ISSN: 0033-7587
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A combination of HPLC and NMR was used to analyze the products of x-irradiated aq. solns. of the dinucleoside monophosphate thymidylyl(3'-5')-2'-deoxyadenosine, d(TpA), and its sequence isomer 2'-deoxyadenylyl(3'-5')thymidine, d(ApT). The products of d(TpA) include both bases and nucleotides and a variety of thymine modifications of d(TpA) including the 2 cis and 2 trans glycol stereoisomers, 2 cis monohydroxy derivs., an N-formamide deriv., and the hydroxymethyl deriv. Attention is focused on using NMR spectral features to distinguish among the various stereoisomers. The radiation chem. of d(ApT) is also explored and differences in product formation compared with d(TpA) are described, particularly the formation of 2 products involving modification of adenine base. The potential of the HPLC-NMR approach to the study of radiation chem. in DNA model compds. is discussed.

IT **102997-98-8**
RL: PROC (Process)
(identification of, as deoxyadenylylthymidine radiolytic product by HPLC and NMR)
RN 102997-98-8 HCAPLUS
CN Thymidine, 2',5'-dideoxy-5',8-cycloadenylyl-(3'.fwdarw.5')- (9CI) (CA

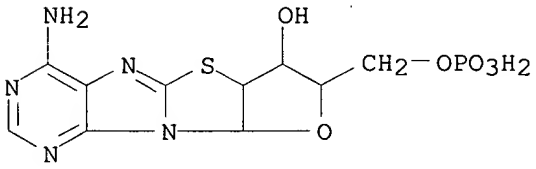
INDEX NAME)



L8 ANSWER 24 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:104570 HCAPLUS
DOCUMENT NUMBER: 104:104570
TITLE: Hydrogen bonding in nucleosides and nucleotides
AUTHOR(S): Jeffrey, G. A.; Maluszynska, H.; Mitra, J.
CORPORATE SOURCE: Dep. Crystallogr., Univ. Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Int. J. Biol. Macromol. (1985), 7(6), 336-48
CODEN: IJBMDR; ISSN: 0141-8130
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An anal. of the H bonding in 76 nucleoside and 11 nucleotide crystal structures shows that the H bond lengths fall into well-defined categories according to the nature of the donor or acceptor groups. The shortest bonds are those involving P-OH or O:P groups. For donor groups, the sequence in bond lengths is P-OH < C-OH < N-H < OW(H)-H < N(H)-H < C-H. There are 10 examples of 2-center bonds. The acceptor sequence is O:P < OH2 < O:C .apprxeq. O(H)C < N .apprxeq. N(H2)C < Cl- < O(C)C < S:C. The no. of 3-center bonds, .apprx.24%, is comparable to that obsd. in the carbohydrates and the amino acids. Most H bonds are involved in short finite chains. Only in the nucleotides are cyclic H bonding schemes obsd.

IT **28220-14-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(hydrogen bonding in)
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



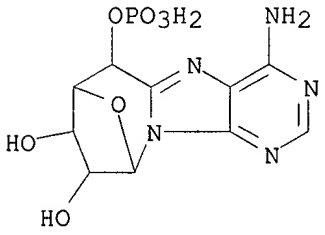
L8 ANSWER 25 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:65065 HCAPLUS
DOCUMENT NUMBER: 104:65065
TITLE: An immunochemical probe for 8,5'-cycloadenosine-5'-monophosphate and its deoxy analog in irradiated nucleic acids

AUTHOR(S): Fuciarelli, A. F.; Miller, G. G.; Raleigh, J. A.
CORPORATE SOURCE: Radiobiol. Cross Cancer Inst., Edmonton, AB, T6G 1Z2, Can.
SOURCE: Radiat. Res. (1985), 104(3), 272-83
CODEN: RAREAE; ISSN: 0033-7587
DOCUMENT TYPE: Journal
LANGUAGE: English

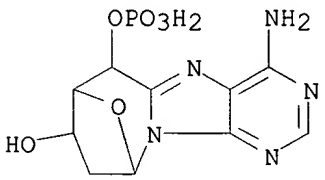
AB Polyclonal antisera specific for 8,5'-cycloadenosine-5'-monophosphate (8,5'-cyclo-AMP) or its deoxy analog (8,5'-cyclo-dAMP) were elicited by immunizing rabbits with a conjugate prepd. by the method of M. I. Johnston et al. (1983). A competitive ELISA was developed and used to detect the formation of these products in irradiated solns. of polyadenylic acid [poly(A)] or DNA which were satd. with nitrous oxide, N, or O. The 8,5'-cyclo-AMP or 8,5'-cyclo-dAMP moieties could be detected in poly(A) at 1.0 krad and in native DNA at 10 krad, resp. The yield of 8,5'-cyclo-dAMP was 2-3-fold higher in irradiated double-stranded DNA than in single-stranded DNA. The hydroxyl radical appears to initiate 8,5'-cyclonucleotide formation in irradiated nucleic acids, as demonstrated by the inhibition of 8,5'-cyclo-AMP formation in irradiated poly(A) by DMSO. However, irradn. under nitrous oxide, particularly at low doses, does not lead to the expected increases in the yield of the 8,5'-cyclonucleotide.

IT **21082-64-4 100217-00-3**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by ELISA after DNA or polyadenylic acid irradn.)

RN 21082-64-4 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate) (8CI, 9CI) (CA INDEX NAME)




RN 100217-00-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8-diol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate) (9CI) (CA INDEX NAME)




L8 ANSWER 26 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1986:16640 HCAPLUS
DOCUMENT NUMBER: 104:16640
TITLE: Hybrid oligomer of cyclonucleotides and deoxynucleotides. A high anti left-handed double helical DNA structure

AUTHOR(S): Uesugi, Seiichi; Lee, Bok Luel; Ikehara, Morio; Kobayashi, Yuji; Kyogoku, Yoshimasa
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, 565, Japan
SOURCE: J. Biomol. Struct. Dyn. (1985), 3(2), 339-47
CODEN: JBSDD6; ISSN: 0739-1102
DOCUMENT TYPE: Journal
LANGUAGE: English

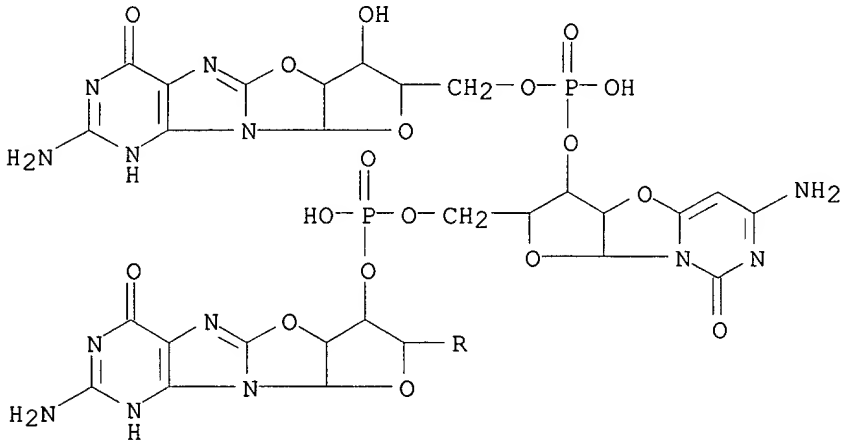
AB It has been shown that oligonucleotides contg. cyclonucleosides with a high anti glycosidic conformation take left-handed, single- and double-helical structures (Uesugi, S., et al., 1977). In order to see whether DNA can adopt the high anti left-handed double helical structure or not, a self-complementary hexanucleotide contg. 6,2'-O-cyclocytidine (Co), 8,2'-O-cycloguanosine (Go), deoxycytidine, and deoxyguanosine, CoGodCdGCoGo, was synthesized. A corresponding hexanucleotide contg. only cyclonucleosides, CoGoCoGoCoGo, was also synthesized. Their conformation was examd. by UV, CD, and 1H NMR spectroscopy. CoGoCoGoCoGo forms an unusually stable, left-handed duplex. Imino proton NMR spectra and the results of nuclear Overhauser effect expts. strongly suggest that CoGodCdGCoGo has a left-handed double helical structure where the deoxynucleoside residues are involved in H bonding and has a high anti glycosidic conformation. Thus, DNA could form a high anti, left-handed double helix which is different from that of Z-DNA under some constrained conditions.

IT **99486-53-0 99499-17-9**
RL: PRP (Properties)
(conformation of)

RN 99486-53-0 HCAPLUS

CN .beta.-D-arabino-Guanosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



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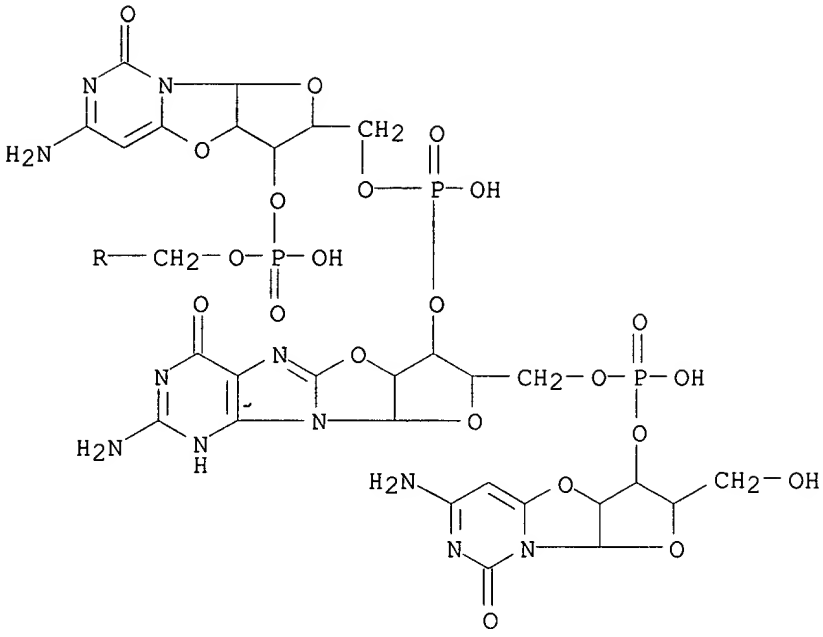
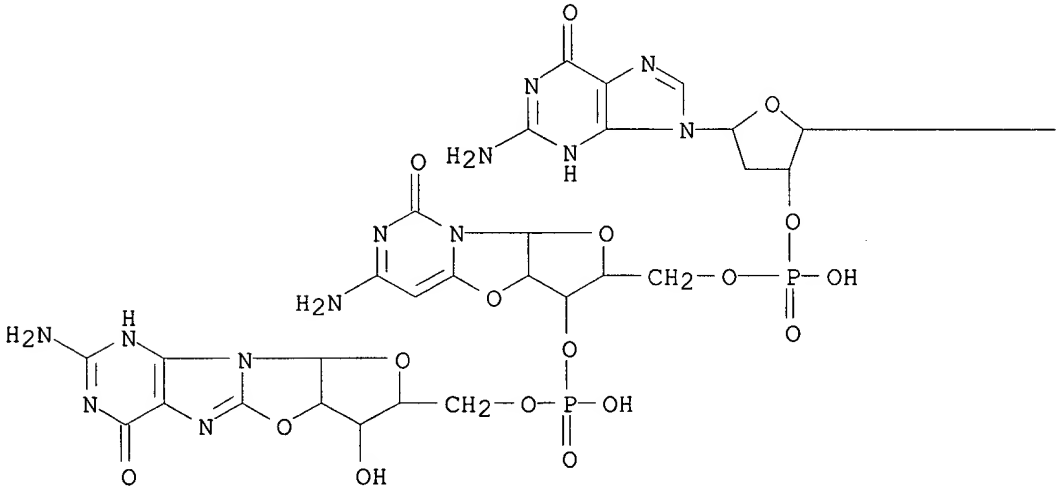
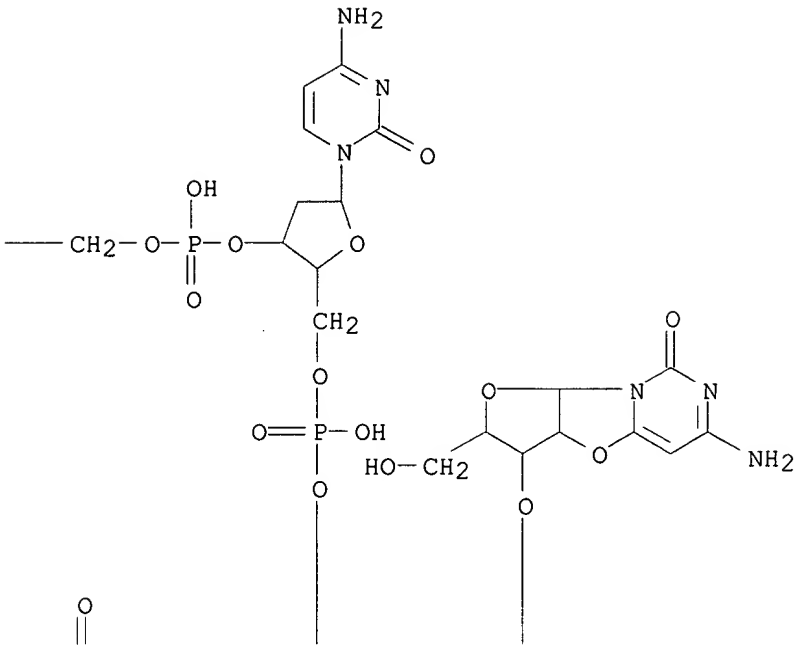


RN 99499-17-9 HCAPLUS
CN .beta.-D-arabino-Guanosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy-.beta.-D-arabino-guanylyl-(3'.fwdarw.5')-2'-deoxycytidylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy-.beta.-D-arabino-cytidylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

PAGE 1-A



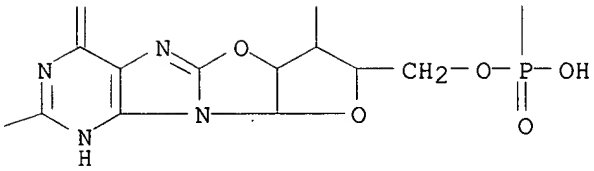
PAGE 1-B



PAGE 2-A

$H_2N$

PAGE 2-B



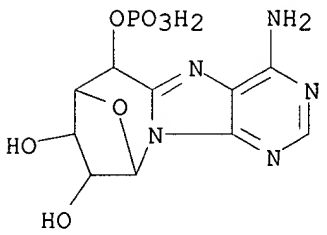
L8 ANSWER 27 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1985:402931 HCAPLUS
DOCUMENT NUMBER: 103:2931
TITLE: Distribution of damage in irradiated 5'-AMP: 8,5'-cyclo-AMP, 8-hydroxy-AMP, and adenine release
AUTHOR(S): Raleigh, J. A.; Fuciarelli, A. F.
CORPORATE SOURCE: Cross Cancer Inst., Edmonton, AB, T6G 1Z2, Can.
SOURCE: Radiat. Res. (1985), 102(2), 165-75

CODEN: RAREAE; ISSN: 0033-7587
DOCUMENT TYPE: Journal
LANGUAGE: English

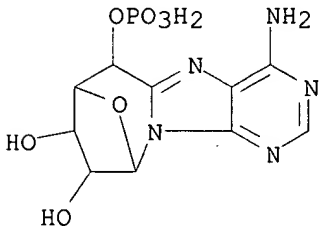
AB The yields of 8,5'-AMP, 8-hydroxy-AMP, and adenine release have been measured in aq. solns. of 5'-AMP, .gamma.-irradiated under N2O. The yields are strongly pH dependent in a way which reflects the pKa's of ionizable groups within 5'-AMP. Redistribution of OH radical attack between base and ribose moieties appears to be occurring in response to changes in the acid-base equil. of 5'-AMP. Other pH-dependent phenomena which only indirectly reflect the pKa's of 5'-AMP include the result that the yield of the (R) epimer of 8,5'-cyclic AMP predominates at low pH whereas that of the (S) epimer predominates at high pH.

IT **41036-59-3 41116-92-1**
RL: RCT (Reactant)
(release of, from AMP after radiolysis in aq. soln. under nitrous oxide atm.)

RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)




RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)



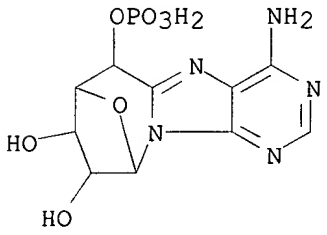

L8 ANSWER 28 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1984:98475 HCAPLUS
DOCUMENT NUMBER: 100:98475
TITLE: Studies on the dynamic syn-anti equilibrium in purine nucleosides and nucleotides with the aid of proton and carbon-13 NMR spectroscopy
AUTHOR(S): Stolarski, Ryszard; Hagberg, Curt Eric; Shugar, David
CORPORATE SOURCE: Inst. Exp. Phys., Univ. Warsaw, Warsaw, PL-02-089, Pol.
SOURCE: Eur. J. Biochem. (1984), 138(1), 187-92
CODEN: EJBCAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal
LANGUAGE: English

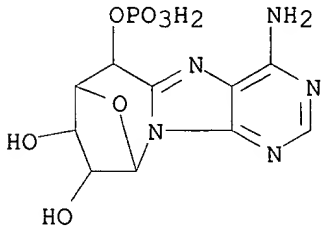
AB Analyses of 1H and 13C NMR spectra have been utilized to extend studies on the dynamic equil. syn-anti about the glycosidic bond of purine nucleosides and nucleotides. With the aid of chem. synthesized model analogs in fixed syn and anti conformations, and the introduction of appropriate corrections for the conformation of the exocyclic chain of the sugar moiety, it is possible to evaluate quant. the relative populations of the syn and anti conformers from the exptl. obsd. chem. shifts of H(2') and C(2'). The resulting agreement between the data based on H(2') chem. shifts with those deduced from C(2') chem. shifts extends the validity of this procedure, and furnishes more accurate results than those previously based on uncorrected H(2') chem. shifts alone. The overall findings are briefly compared with those derived from measurements of proton relaxation times and the Overhauser effect, as well as by x-ray diffraction in the solid state. Attention is drawn to the potential utility of the results, including chem. shift data, in studies on interactions of nucleosides and nucleotides with appropriate enzyme systems.

IT **41036-59-3 41116-92-1**
RL: PRP (Properties)
(NMR of, conformational equil. in relation to)

RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)




RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)




L8 ANSWER 29 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1983:179814 HCAPLUS
DOCUMENT NUMBER: 98:179814
TITLE: NMR lanthanoid-probe analyses of conformational properties of 8,2'-S-cycloadenosine 3'-monophosphate in aqueous solution

AUTHOR(S): Yokoyama, Shigeyuki; Oida, Tetsuya; Uesugi, Seiichi; Ikehara, Morio; Miyazawa, Tatsuo
CORPORATE SOURCE: Fac. Sci., Univ. Tokyo, Tokyo, 113, Japan
SOURCE: Bull. Chem. Soc. Jpn. (1983), 56(2), 375-8
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
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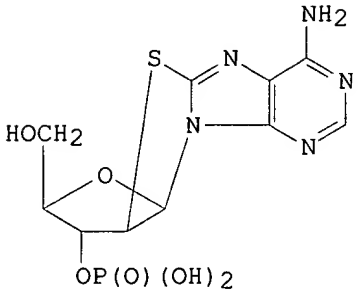


I

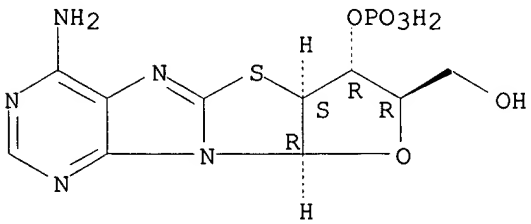
AB The advanced method of NMR lanthanoid-probe analyses was used for studying the mol. conformations of I in aq. soln. From the obsd. ratios of Pr(III)-induced shifts, Gd(III)-enhanced relaxation rates as well as vicinal spin-coupling consts., the most probable values (and std. deviations) of the fractional populations of the local conformations for the C5'-C4' bond, sugar ring, C3'-O3' bond, and O3'-P bond and the internal rotation angles of the two forms about the C3'-O3' bond were detd. by the program COFLEM. The internal rotation equil. about the C3'-O3' bond was found to be interrelated with the puckering of the sugar ring. The advance lanthanoid probe method is thus useful for the analyses of the conformational characteristics of cyclonucleotides as well as of unmodified nucleotides in aq. soln.

IT **55652-02-3**
RL: PRP (Properties)
(conformation of, NMR lanthanoid-probe anal. of)

RN 55652-02-3 HCAPLUS

CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



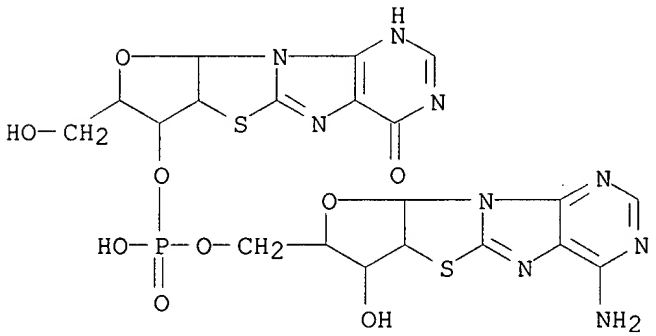
L8 ANSWER 30 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:572837 HCAPLUS
DOCUMENT NUMBER: 97:172837

TITLE: Structure of a dinucleoside monophosphate having a high anti configuration. II. Structure of 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosylhypoxanthylyl(3'-5')-8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine (IspAs) hexahydrate
AUTHOR(S): Hamada, Kensaku; Matsuo, Yoshiko; Miyamae, Akira; Fujii, Satoshi; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan
SOURCE: Acta Crystallogr., Sect. B (1982), B38(9), 2528-31
CODEN: ACBCAR; ISSN: 0567-7408
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The title compd. is triclinic, space group P1, with a 14.324(5), b 11.130(3), c 5.794(1) .ANG., .alpha. 97.40(3), .beta. 87.42(3), and .gamma. 120.05(4).degree.; dm = 1.630(1) and dc = 1.536 for Z = 1. The final R is 0.066. The at. parameters and bond lengths and angles are given. The mol. conformation is a folded form, with (g+,t) torsion angles around P-O bonds, which is stabilized by hydrophobic interactions between sugar and base moieties and by intermol. base stacking.

IT **83376-33-4**
RL: PRP (Properties)
(structure of)

RN 83376-33-4 HCAPLUS
CN Phosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] mono[1,4,6a,7,8,9a-hexahydro-8-(hydroxymethyl)-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-7-yl] ester, hexahydrate, stereoisomer (9CI) (CA INDEX NAME)

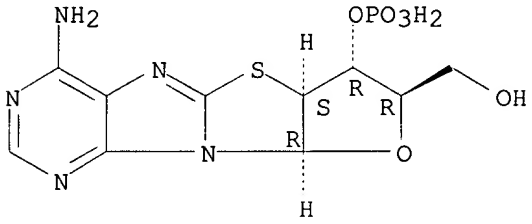


● 6 $H_2O$

L8 ANSWER 31 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:518459 HCAPLUS
DOCUMENT NUMBER: 97:118459
TITLE: Structural studies of S-cycloadenosine derivatives. III. The structure of 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine 3'-monophosphate (Asp)
AUTHOR(S): Miyamae, Akira; Tanaka, Kaori; Hamada, Kensaku; Fujii, Satoshi; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, 565, Japan

SOURCE: Acta Crystallogr., Sect. B (1982), B38(7), 1937-42
CODEN: ACBCAR; ISSN: 0567-7408
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure of the title compd. was detd. by direct methods and refined to an R of 0.059 for 2779 reflections. The crystals, are monoclinic, space group P21, with a 11.239(1), b 11.564(1), c 13.058((2) .ANG., and .beta. 110.25(1).degree.; dc = 1.585 and do = 1.581(3) for Z = 2. The confirmations of the 2 independent mols. (A and B) are similar except for the orientation of the PO4 group, which agrees with the conformations obsd. in soln. by NMR. Both sugar puckerings are C(4')-endo, the orientations of C(5')-O(5') are gauche-trans and the torsion angles are 191.9(6) (A) and 255.4(7).degree. (B). At. coordinates are given.
IT **82890-28-6**
RL: PRP (Properties)
(structure of)
RN 82890-28-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, dihydrate, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




●2 $H_2O$

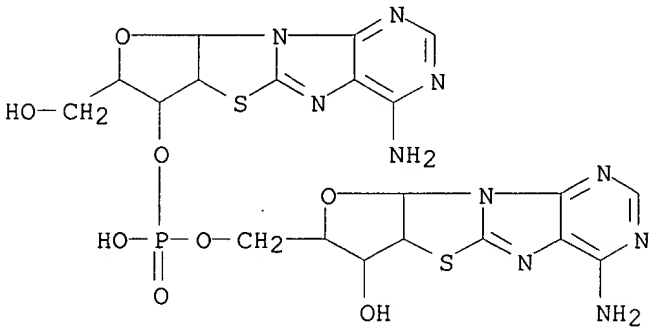
L8 ANSWER 32 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1982:133619 HCAPLUS
DOCUMENT NUMBER: 96:133619
TITLE: The structure of a dinucleoside monophosphate having a high-anti conformation: 8,2'-S-cyclo-2'-thioadenylyl(3'-5')-8,2'-S-cyclo-2'-thioadenosine (AspAs) hydrochloride
AUTHOR(S): Fujii, Satoshi; Hamada, Kensaku; Miura, Reiko; Uesugi, Seiichi; Ikehara, Morio; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, 565, Japan
SOURCE: Acta Crystallogr., Sect. B (1982), B38(2), 564-70
CODEN: ACBCAR; ISSN: 0567-7408
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title structure was refined to an R of 0.078. AspAsis triclinic, space group P1, with a 11.161(4), b 11.824(4), c 12.136(3) .ANG., .alpha. 89.20(3), .beta. 97.92(3), and .gamma. 116.75(2).degree.; Z = 1 for, dm = 1.655(4) and, dc = 1.65. The mol. conformations of 2 independent AspAsmols. in an asym. unit are almost identical, and are both in the sharp "bend" conformation, i.e. the rotation (.omega.',.omega.) around the P-O bond is (g-,t) rather than the preferred (g-,g-) or (g1,g1). These torsion angles concerning the sugar-phosphate backbone are quite distinct

from those found in cryst. dinucleoside monophosphates. There is no intramol. base stacking or base pairing but strong intermol. base stacking exists. At. coordinates are given.

IT **81245-03-6**
RL: PRP (Properties)
(structure of)

RN 81245-03-6 HCAPLUS

CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-, monohydrochloride, hydrate (9CI) (CA INDEX NAME)



● HCl

● x $H_2O$

L8 ANSWER 33 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:569660 HCAPLUS

DOCUMENT NUMBER: 95:169660

TITLE: Studies of nucleosides and nucleotides. 36. Synthesis of 5'-deoxy-8,5'-cycloguanosine 2',3'-cyclic phosphate and 3'-phosphate and their interaction with ribonuclease T1

AUTHOR(S): Matsuda, Akira; Ueda, Tohru

CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Sapporo, 060, Japan

SOURCE: Nippon Kagaku Kaishi (1981), (5), 845-50
CODEN: NKAKB8; ISSN: 0369-4577

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

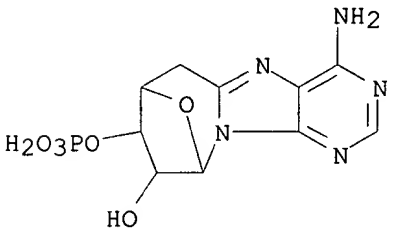
AB Photocyclization of 5'-deoxy-5'-(phenylthio)guanosine 2',3'-cyclic phosphate furnished 5'-deoxy-8,5'-cycloguanosine 2',3'-cyclic phosphate, a fixed model of the anti-form of guanosine 2',3'-cyclic phosphate, which was digestible with RNase T1 to give the 3'-phosphate. The spectral anal. of the interaction of RNase T1 and the 8,5'-cycloguanosine 3'-phosphate revealed that it behaved exactly like 3'-guanylate. The previous assumption of interaction between RNase T1 and guanosine 3'-phosphate of syn form has now been revised, since the cycloguanine nucleotide should possess the anti-form. The corresponding adenine nucleotide was also synthesized.

IT **79431-87-1P**

RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in digestion of deoxycycloguanosine cyclic phosphate by RNase T1)

RN 79431-87-1 HCAPLUS

CN 7,10-Epoxy-6H-azepino[1,2-e]purine-8,9-diol, 4-amino-7,8,9,10-tetrahydro-, 8-(dihydrogen phosphate), [7R-(7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)




L8 ANSWER 34 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1981:492537 HCAPLUS

DOCUMENT NUMBER: 95:92537

TITLE: Effect of sequence on the spatial configuration of high anti nucleic acids and evidence for left-handed double helixes

AUTHOR(S): Dhingra, M. M.; Sarma, Ramaswamy H.; Uesugi, S.; Shida, T.; Ikehara, M.

CORPORATE SOURCE: Inst. Biomol. Stereodyn., State Univ. New York, Albany, NY, 12222, USA

SOURCE: Biochemistry (1981), 20(17), 5002-11
CODEN: BICHAW; ISSN: 0006-2960

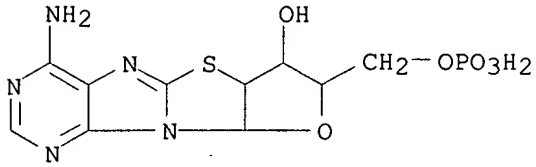
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The conformational properties of pyrimidine-purine and pyrimidine-purine dinucleoside monophosphates in which the glycosidic torsion is fixed to .simeq.120.degree. by formation of a covalent link between the base and the sugar ring are explored by 1H NMR spectroscopy in order to obtain information about the spatial configuration of high anti nucleic acids. The intramol. stack of the high anti dimers were left-handed, in contrast to that (right-handed) for natural oligomers, which are low anti. Even though both the high anti pyrimidine-purine and purine-pyrimidine dimers have similar backbone torsion angles, they display widely different relative geometry between the bases; thus, in the former there is extensive base-base overlap in the stack, and in the latter there is negligible intramol. base-base overlap. In addn., purine-pyrimidine systems form miniature double helixes in which there is substantial interstrand purine-purine interaction; on the other hand the pyridine-purine high anti dinucleosides have no proclivity to form such-paired complexes in soln. Math. polymn. of the conformation of the high anti purine-pyrimidine dinucleoside monophosphates generates a left-handed helix for high anti polynucleotides. This also means that the double helix for high anti nucleic acids contg. purine-pyrimidine repeating units may also be left handed but one of its principal features will be interstrand base stacking. It is suggested that the plasticity in the structure of genomic DNA is such that, if under certain conditions of interactions the sugar-base torsion of certain domains assume high anti values, that domain will become left handed, and this in turn can be a mechanism for the control of expression by genomic DNA.

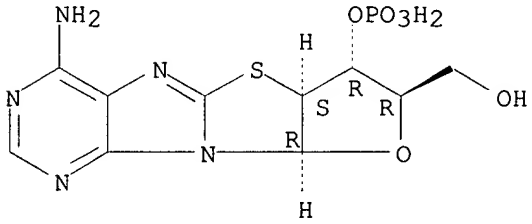
IT **28220-14-6 55652-02-3**

RL: PRP (Properties)
(NMR of)
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

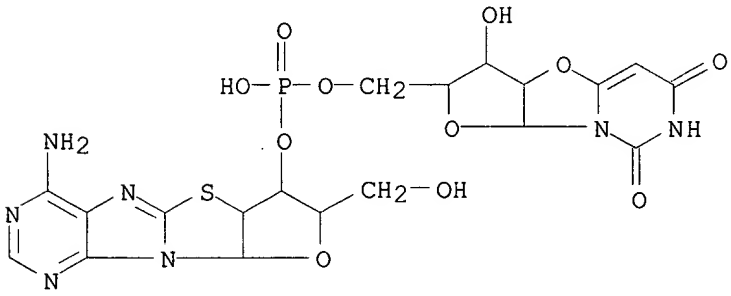


RN 55652-02-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

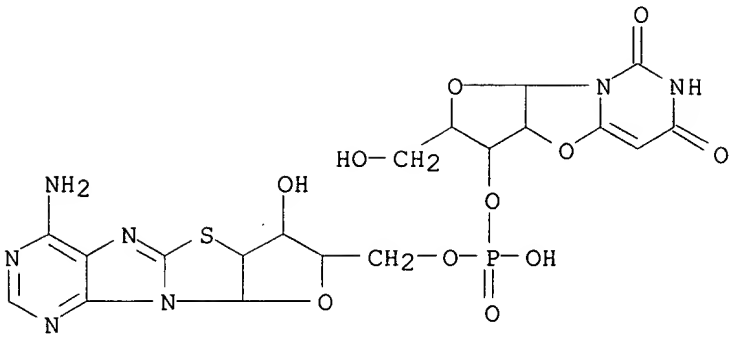
Absolute stereochemistry.



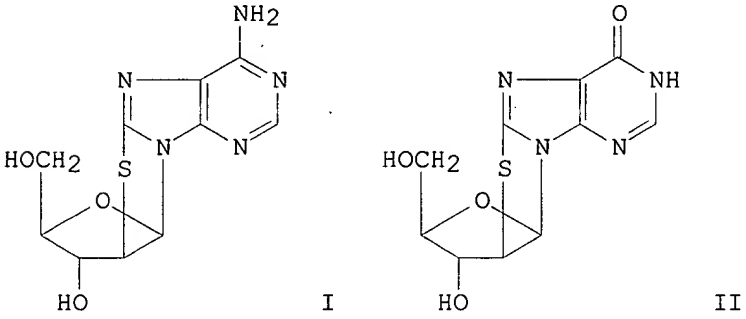
IT **73705-78-9 73705-79-0**
RL: PRP (Properties)
(conformation of, high anti nucleic acids in relation to)
RN 73705-78-9 HCAPLUS
CN .beta.-D-arabino-Uridine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)



RN 73705-79-0 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-uridylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



L8 ANSWER 35 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:443540 HCAPLUS
DOCUMENT NUMBER: 95:43540
TITLE: Polynucleotides. LXI. Synthesis and properties of dinucleoside monophosphates containing 8,2'-S-cycloadenosine and 8,2'-S-cycloinosine residues. Sequence dependency of the stability of the stacking conformation
AUTHOR(S): Uesugi, Seiichi; Shida, Toshio; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan
SOURCE: Chem. Pharm. Bull. (1980), 28(12), 3621-31
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

AB Three dinucleoside monophosphates contg. 8,2'-anhydro-8-thio-9-.beta.-D-arabinofuranosyladenine (AS, I) and its hypoxanthine deriv. (IS, II), ASpIS, ISpAS and ISpIS, were prepd. Examn. of their UV, CD, and 1H-NMR spectra and comparison with the properties of ASpAS, which has been shown to take a left-handed stacked conformation, showed that all these dimers take a left-handed stacked conformation, and the order of extent of stacking is ASpAS.apprxeq.ISpAS.apprxeq.ISpIS. This sequence dependency of stability of stacking can be explained in terms of the mode of base-base overlap in a left-handed stack. A similar explanation may be applicable to the corresponding sequence dependency of natural dimers with a right-handed stack.

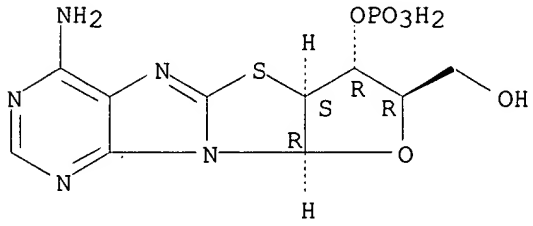
IT **78086-10-9**
RL: RCT (Reactant)

(benzylation of)
RN 78086-10-9 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, compd. with pyridine (9CI) (CA INDEX NAME)

CM 1

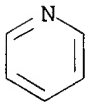
CRN 55652-02-3
CMF C10 H12 N5 O6 P S
CDES *

Absolute stereochemistry.




CM 2

CRN 110-86-1
CMF C5 H5 N

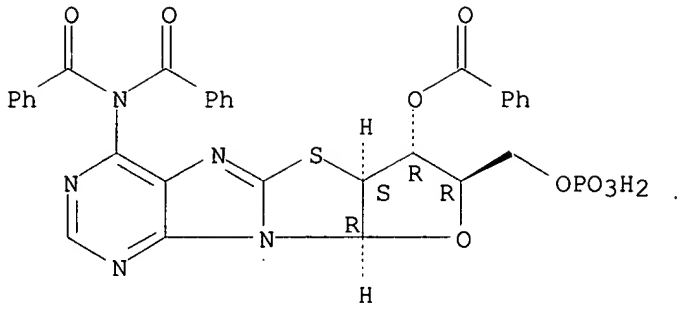



IT **78039-47-1**
RL: RCT (Reactant)
(coupling reaction of, with cycloinosine deriv.)
RN 78039-47-1 HCAPLUS
CN Benzamide, N-benzoyl-N-[7-(benzoyloxy)-6a,7,8,9a-tetrahydro-8-[(phosphonooxy)methyl]furo[2',3':4,5]thiazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, compd. with pyridine (9CI) (CA INDEX NAME)

CM 1

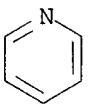
CRN 73715-15-8
CMF C31 H24 N5 O9 P S
CDES *

Absolute stereochemistry.

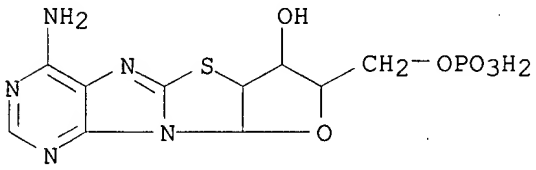


CM 2

CRN 110-86-1
CMF C5 H5 N



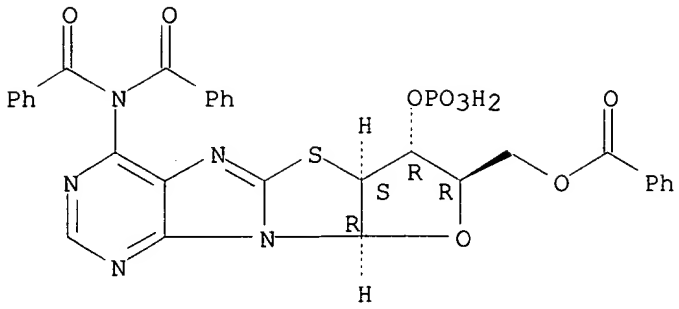
IT **78086-09-6**
RL: RCT (Reactant)
(deamination of)
RN 78086-09-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), sodium salt, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



●x Na

IT **78007-78-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and coupling reaction of, with cycloinosine deriv.)
RN 78007-78-0 HCAPLUS
CN Benzamide, N-benzoyl-N-[8-[(benzoyloxy)methyl]-6a,7,8,9a-tetrahydro-7-(phosphonooxy)furo[2',3':4,5]thiazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

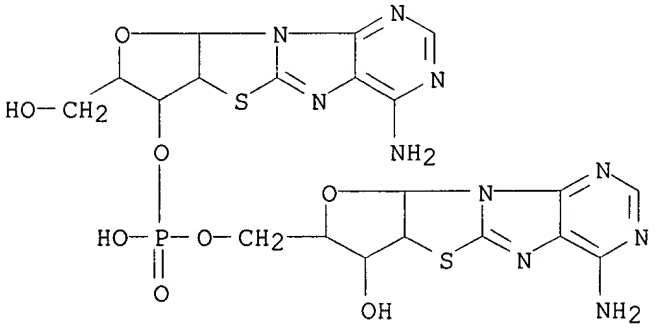
Absolute stereochemistry.



IT **78039-48-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deamination of)
RN 78039-48-2 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-7-[[[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methoxy]hydroxyphosphinyl]oxy]-6a,7,8,9a-tetrahydro-, [6aS-[6a.alpha.,7.alpha.(6aR*,7S*,8S*,9aS*),8.beta.,9a.alpha.]]-, compd. with N,N-diethylethanamine (9CI) (CA INDEX NAME)

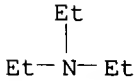
CM 1

CRN 29617-82-1
CMF C20 H21 N10 O8 P S2
CDES *



CM 2

CRN 121-44-8
CMF C6 H15 N

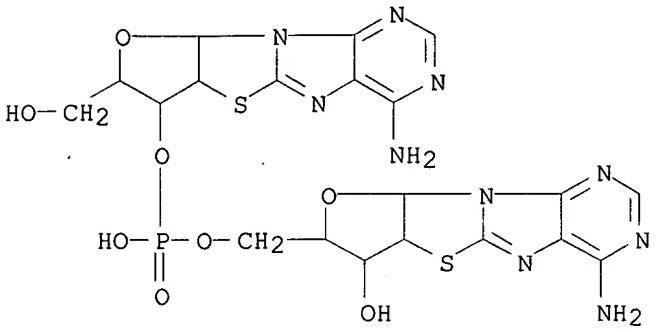


IT **29617-82-1P 50271-86-8P 76385-12-1P**
**78000-53-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and stacking conformation of)

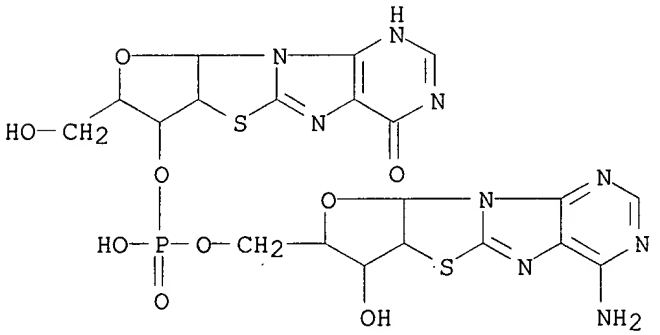
RN 29617-82-1 HCAPLUS

CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



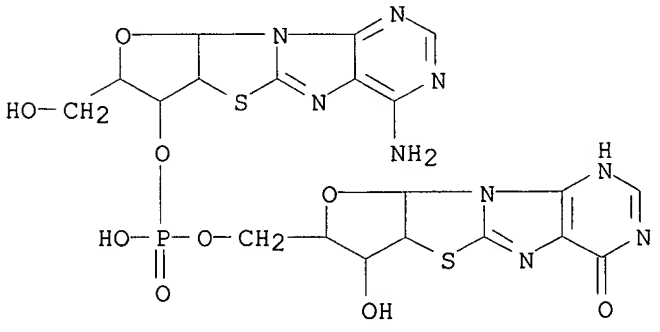
RN 50271-86-8 HCAPLUS

CN Phosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] mono[1,4,6a,7,8,9a-hexahydro-8-(hydroxymethyl)-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-7-yl] ester, stereoisomer (9CI) (CA INDEX NAME)

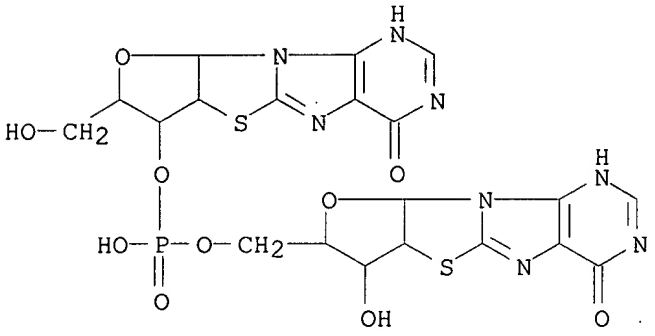


RN 76385-12-1 HCAPLUS

CN Arainosine, 2'-deoxy-2',8-epithioaraadenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)

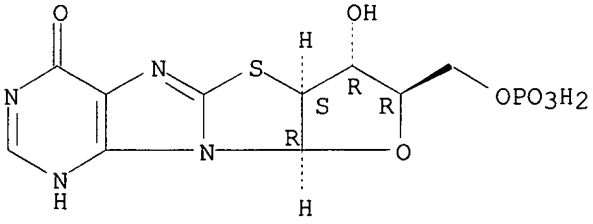


RN 78000-53-0 HCAPLUS
CN Arainosine, 2'-deoxy-2',8-epithioarainosinylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



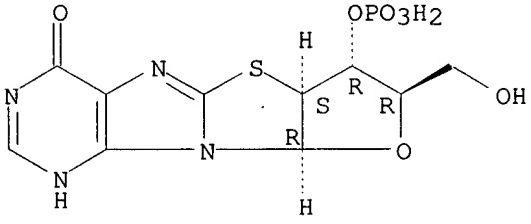
IT **50458-24-7P 78007-77-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 50458-24-7 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purin-4(3H)-one, 6a,7,8,9a-tetrahydro-7-hydroxy-8-[(phosphonooxy)methyl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 78007-77-9 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purin-4(1H)-one, 6a,7,8,9a-tetrahydro-8-(hydroxymethyl)-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



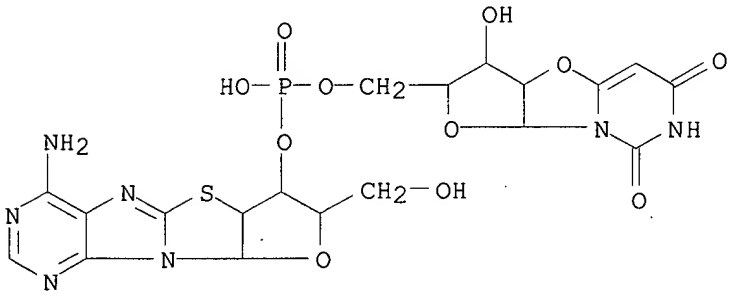
L8 ANSWER 36 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:438353 HCAPLUS

DOCUMENT NUMBER: 95:38353
TITLE: Solution structure of DNA: the method of nuclear magnetic resonance spectroscopy
AUTHOR(S): Mitra, C. K.; Sarma, Ramaswamy H.; Giessner-Prettre, C.; Pullman, Bernard
CORPORATE SOURCE: Inst. Biomol. Stereodyn., State Univ. New York, Albany, NY, USA
SOURCE: Int. J. Quantum Chem., Quantum Biol. Symp. (1980), 7, 39-66
CODEN: IJQBDZ; ISSN: 0360-8832
DOCUMENT TYPE: Journal
LANGUAGE: English

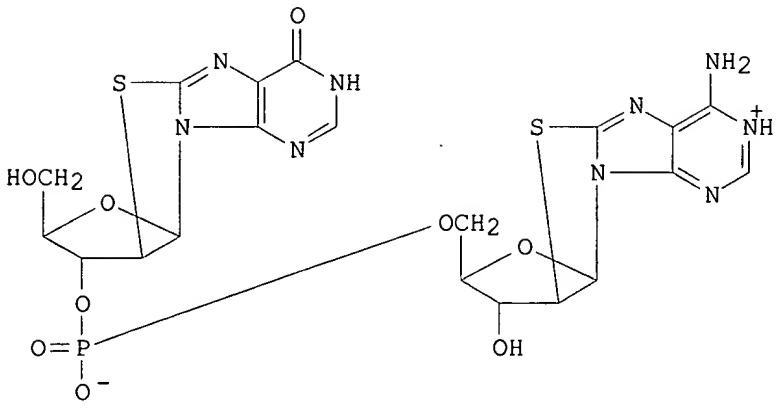
AB A method of NMR spectroscopy which involves the computation of magnetic shielding consts. from xyz coordinates taking into consideration the contribution to shielding from ring current fields, the diamagnetic and paramagnetic components of the at. magnetic anisotropy, is presented to solve the soln. spatial configuration of single-stranded and double-helical nucleic acids. Apparently, the CCA terminus of tRNA in soln. assumes a structure very much different from its crystal structure. However, for the double-helical poly(dG-DC).cntdot.poly(dG-dC) in high salt soln., the obsd. structure shows eminent agreement with the left-handed Z-DNA proposed from single crystal structural studies.

IT **73705-78-9**
RL: ANST (Analytical study)
(double stranded, structure of, in soln., NMR of)

RN 73705-78-9 HCAPLUS
CN .beta.-D-arabino-Uridine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)



L8 ANSWER 37 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:209116 HCAPLUS
DOCUMENT NUMBER: 94:209116
TITLE: Dinucleoside monophosphate having a high anti conformation. II. The crystal structure of 8,2'-S-cycloinosinyl-(3',5')-8,2'-S-cycloadenosine hexahydrate
AUTHOR(S): Hamada, Kensaku; Matsuo, Yoshiko; Miyamae, Akira; Fujii, Satoshi; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, 565, Japan
SOURCE: Nucleic Acids Symp. Ser. (1980), 8, s157-s160
CODEN: NACSD8
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



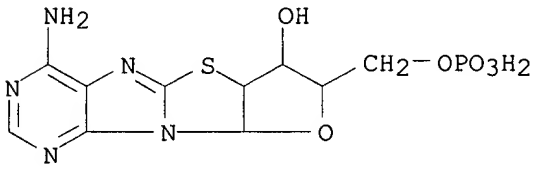
I

AB The crystal and mol. structure of the title nucleotide (I) hexahydrate was detd. by x-ray diffraction method. The torsion angles around the sugar-phosphate backbone are unique and different from those in the cryst. dinucleoside monophosphates so far detd. The rotation around the P-O bond, (.omega.',.omega.), is (g+,t). I mol. is in a folded form. There is no intramol. base stacking or base-pairing but the intermol. base stacking is dominant.

IT **28220-14-6**
RL: RCT (Reactant)
(condensation reaction of, with S-cycloinosine)

RN 28220-14-6 HCAPLUS

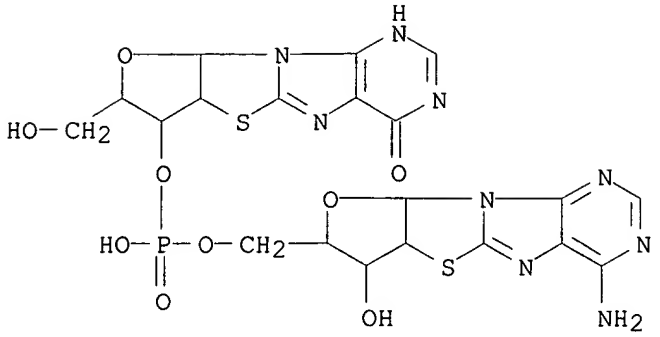
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



IT **50271-86-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal and mol. structure of)

RN 50271-86-8 HCAPLUS

CN Phosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] mono[1,4,6a,7,8,9a-hexahydro-8-(hydroxymethyl)-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-7-yl] ester, stereoisomer (9CI) (CA INDEX NAME)

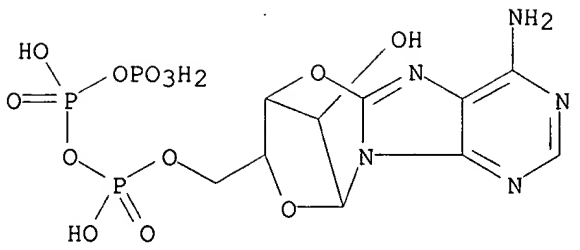


L8 ANSWER 38 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:170088 HCAPLUS
DOCUMENT NUMBER: 94:170088
TITLE: Chemically modified ATP derivatives for the study of aminoacyl-tRNA synthetases from Bakers' yeast: ATP analogs with fixed conformations of modified triphosphate chains in the aminoacylation reaction
AUTHOR(S): Freist, Wolfgang; Wiedner, Harald; Cramer, Friedrich
CORPORATE SOURCE: Abt. Chem., Max-Planck-Inst. Exp. Med., Goettingen, D-34, Fed. Rep. Ger.
SOURCE: Bioorg. Chem. (1980), 9(4), 491-504
CODEN: BOCMBM; ISSN: 0045-2068
DOCUMENT TYPE: Journal
LANGUAGE: English

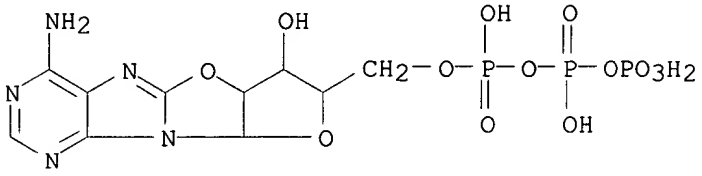
AB A systematic investigation of the substrate specificity of aminoacyl-tRNA synthetases from yeast was completed by tests of ATP analogs with fixed conformation about the glycosidic bond and with modifications in the triphosphate chain as substrate analogs in the aminoacylation reaction. Two analogs with fixed high anti (8,2'-O-cyclo-ATP, 8,2'-S-cyclo-ATP) and 2 with fixed anti (8,3'-O-cyclo-ATP, 8,3'-S-cyclo-ATP) conformation were tested in the esterification reaction of phenylalanyl-, seryl-, lysyl-, valyl-, isoleucyl-, arginyl-, and tyrosyl-tRNA synthetases from bakers' yeast. None of the compds. was a substrate, whereas 11 Ki values could be detd. All the synthetases were inhibited by 8,2'-S-cyclo-ATP. Each compd. with a fixed anti conformation inhibits 2 enzymes. Among 11 analogs with modifications in the triphosphate chain, 4 were substrates for phenylalanyl-, 3 for seryl-, 1 for lysyl-, 3 for valyl-, 1 for isoleucyl-, and none for arginyl- or tyrosyl-tRNA synthetases. Two compds. were inhibitors of different types for phenylalanyl-, 2 for seryl-, 7 for lysyl-, 6 for valyl-, 9 for isoleucyl-, 7 for arginyl-, and 2 for tyrosyl-tRNA synthetases. Their Km, Vmax, and Ki values were detd. In general, the subunit enzymes can tolerate substitutions in positions 2, 2', the .alpha.-P, the .beta.,.gamma.-phosphate bridge, and at the .gamma.-P atom. The single-chain enzymes tolerate substitutions at position 7 and at the .gamma.-P. All 7 synthetases from yeast need an intact NH2 group in position 6 and an O in position 3'.

IT **68299-75-2P 68299-76-3P 68745-46-0P 68745-47-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and aminoacyl-tRNA synthetase specificity for)

RN 68299-75-2 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]dioxazepino[3,2-e]purin-8-yl)methyl] ester, [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)

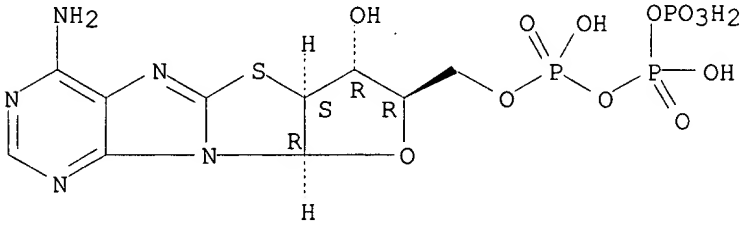


RN 68299-76-3 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]oxazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

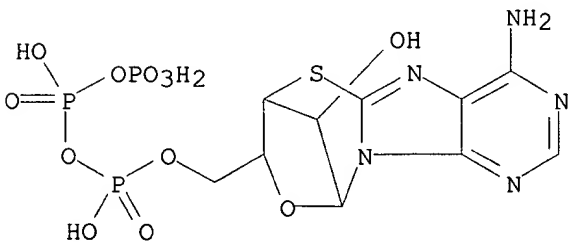


RN 68745-46-0 HCAPLUS
CN Triphosphoric acid, P-[[(6aS,7R,8R,9aR)-4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

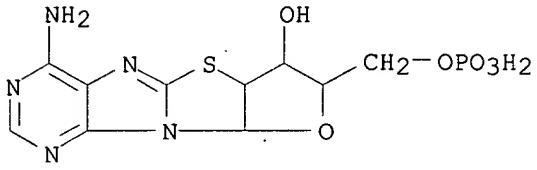


RN 68745-47-1 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-8-yl)methyl] ester, [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)

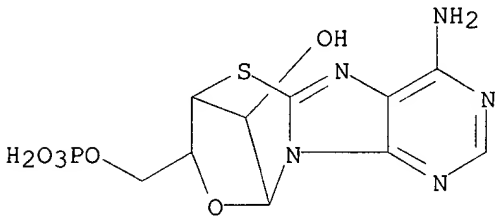


IT **28220-14-6P 35782-70-8P 42582-26-3P**
**42735-42-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphorylation of)

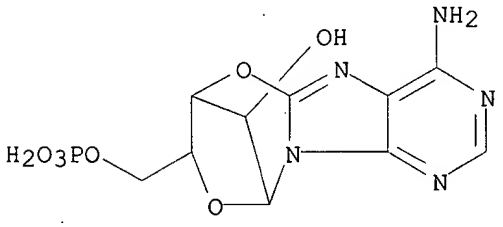
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



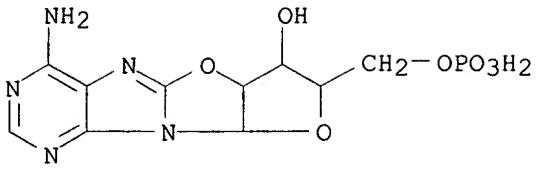
RN 35782-70-8 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)



RN 42582-26-3 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]dioxazepino[3,2-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)



RN 42735-42-2 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

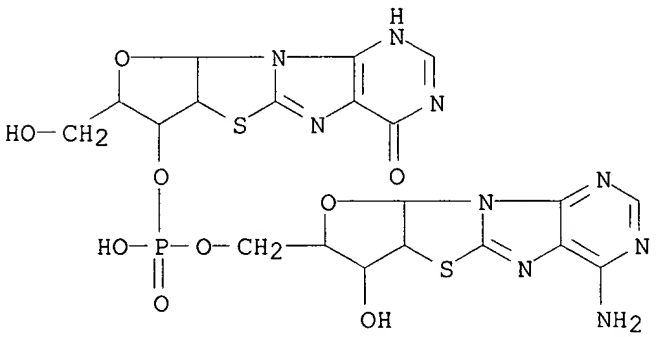


L8 ANSWER 39 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:60022 HCAPLUS
DOCUMENT NUMBER: 94:60022
TITLE: Interactions between oligonucleotides having a left-handed helical structure and ethidium bromide
AUTHOR(S): Uesugi, Seiichi; Shida, Toshio; Miyamae, Akira; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, 565, Japan
SOURCE: Nucleic Acids Symp. Ser. (1980), 8, s147-s150
CODEN: NACSD8
DOCUMENT TYPE: Journal
LANGUAGE: English

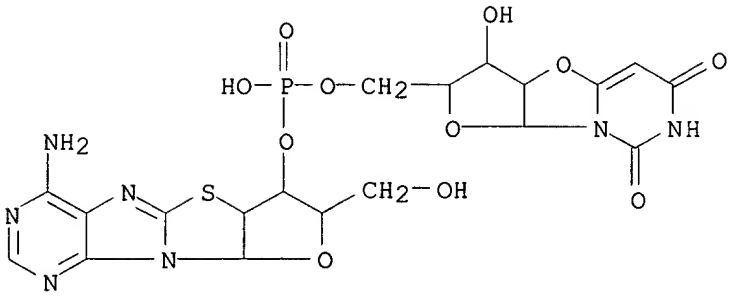
AB Oligonucleotides contg. 8,2'-S-cycloadenosine (As), 8,2'-S-cycloinosine (Is), 6,2'-O-cyclouridine (U.degree.), and 6,2'-O-cyclocytidine (C.degree.) residues, which have a glycosidic torsion angle .apprx.120.degree., were synthesized. Among these oligomers, AspU.degree., AspIs, and (pC.degree.)4 + (pIs)4 formed a complex with ethidium bromide which was assumed to be intercalated between the adjacent base-pairs of the left-handed double helix.

IT **50271-86-8 73705-78-9 73705-79-0**
**76385-12-1 76466-22-3**
RL: BIOL (Biological study)
(ethidium bromide interaction with)

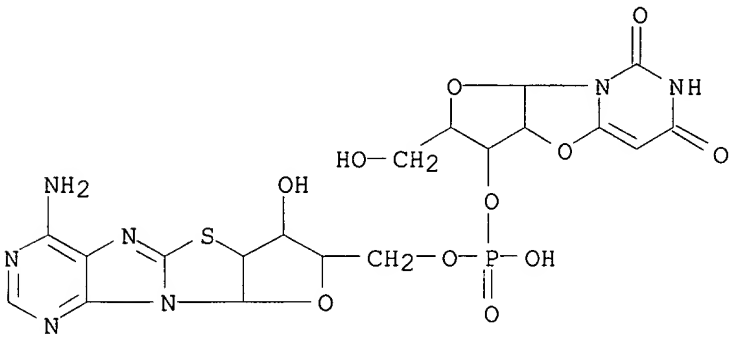
RN 50271-86-8 HCAPLUS
CN Phosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] mono[1,4,6a,7,8,9a-hexahydro-8-(hydroxymethyl)-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-7-yl] ester, stereoisomer (9CI) (CA INDEX NAME)



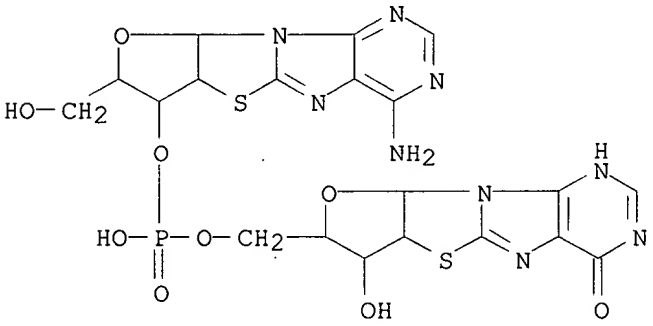
RN 73705-78-9 HCAPLUS
CN .beta.-D-arabino-Uridine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)



RN 73705-79-0 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-uridylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



RN 76385-12-1 HCAPLUS
CN Arainosine, 2'-deoxy-2',8-epithioaraadenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



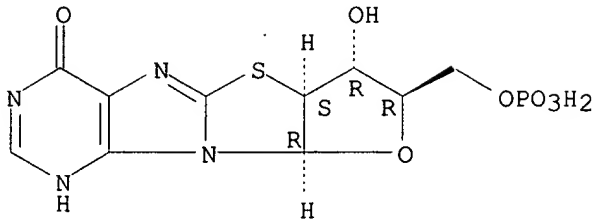
RN 76466-22-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purin-4(1H)-one, 6a,7,8,9a-tetrahydro-7-hydroxy-8-[(phosphonooxy)methyl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

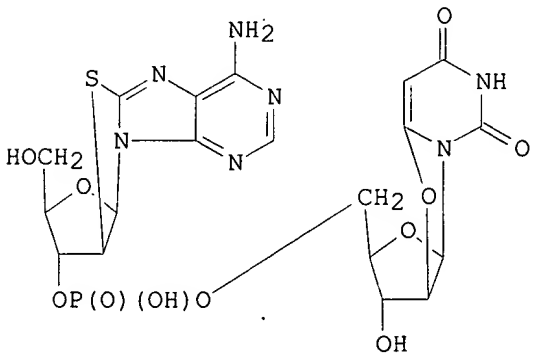
CRN 50458-24-7
CMF C10 H11 N4 O7 P S

CDES *

Absolute stereochemistry.



L8 ANSWER 40 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1981:26273 HCAPLUS
DOCUMENT NUMBER: 94:26273
TITLE: Experimental support for a right-handed vertical double helix
AUTHOR(S): Mitra, C. K.; Dhingra, M. M.; Sarma, Ramaswamy H.
CORPORATE SOURCE: Inst. Biomol. Stereodyn., State Univ. New York, Albany, NY, 12222, USA
SOURCE: Biopolymers (1980), 19(8), 1435-50
CODEN: BIPMAA; ISSN: 0006-3525
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



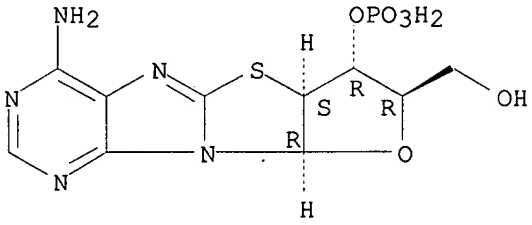
I

AB The exptl. obsd. geometry of a miniature double helix of high anti (.chi.CN fixed .simeq.120.degree., with .chi.CN being the glycosidic torsion angle) nucleic acid structure indicates substantial interstrand base stacking with little intrastrand base stacking. This geometry is consistent with the right-handed vertical double helix in which the base planes are parallel to helical axis, as proposed by W. K. Olson (1977) from theor. calcns. The exptl. data do not agree with the left-handed model in which the base planes are perpendicular to the helical axis, as proposed by N. Yathindra and M. Sundaralingam (1976). The theor. computed chem. shift changes for the various double-helical configurations show that, for the system examd., only the vertical model can explain the exptl. obsd. shift trends. The melting curve for the helix-coil transition for a high anti cyclodinucleoside monophosphate (I) has been obsd. for the 1st time. Even though the exptl. data support vertical

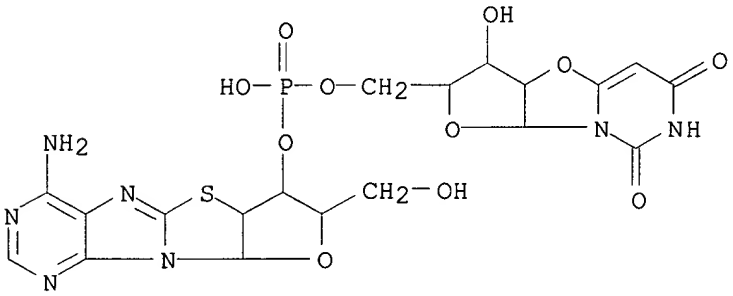
double helices when .chi.CN is fixed at 120.degree., data on naturally occurring nucleic acid structures indicate that they have no proclivity to enter into vertically stabilized double-helical arrays.

IT **55652-02-3**
RL: BIOL (Biological study)
(NMR of,)
RN 55652-02-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

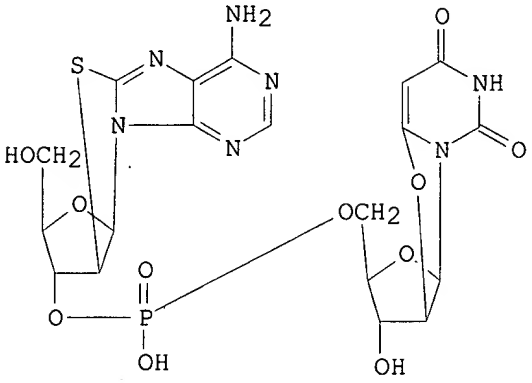



IT **73705-78-9**
RL: BIOL (Biological study)
(hydrogen-bonded dimer, vertical double-helical conformation of, NMR in relation to)
RN 73705-78-9 HCAPLUS
CN .beta.-D-arabino-Uridine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 41-61

L8 ANSWER 41 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:599415 HCAPLUS
DOCUMENT NUMBER: 93:199415
TITLE: Is DNA really a double helix? Its diverse spatial configurations and the evidence for a vertically stabilized double helix
AUTHOR(S): Sarma, Ramaswamy H.
CORPORATE SOURCE: Inst. Biomol. Stereodyn., State Univ. New York, Albany, NY, 12222, USA
SOURCE: Nucleic Acid Geom. Dyn. (1980), 83-108, 16 plates. Editor(s): Sarma, Ramaswamy H. Pergamon: Elmsford, N. Y.
CODEN: 43XVAF
DOCUMENT TYPE: Conference
LANGUAGE: English
GI

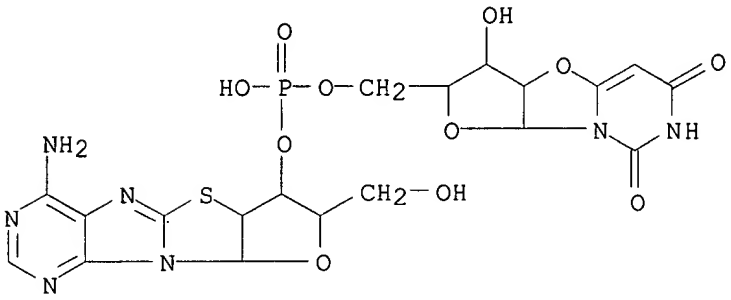


I

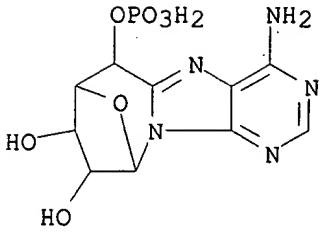
AB Extensive literature data on the structure of DNA is discussed in terms of the helical organization of single- and double-stranded high anti polynucleotides. The cyclodinucleoside monophosphate AspU.degree. (I) was studied by 1H NMR as a nucleic acid constituent with a sugar base torsion angle of .apprx.120.degree. and which can form double-helical helixes. The chem. shift of the base proton H2 of the Asp- segment of I moved markedly upfield relative to the corresponding proton in the mononucleotide Asp, whereas the chem. shift of the uridine H5 was little affected. The concn. dependence of the chem. shifts of I further suggest that the rigid high anti .chi.CN of .apprx.120.degree. in I renders the easy formation of a double helix stabilized by adenine-adenine interactions. Helix-coil transition in I was obsd. from melting effects on the adenine H2 chem. shifts and thermodn. parameters were calcd. Evidently, I forms miniature double helixes with significant interstrand and little intrastrand base-base interactions. These results render untenable the rigid nucleotide, left-handed model of M. Sundaralingam and N. Yathindra (1976) and support the novel vertical double helix for high anti polynucleotides (Olson, W. K., 1977). Self-complementary ApU and d(pGpC) appear to have no potentiality to form such miniature double helixes.

IT **73705-78-9**
RL: BIOL (Biological study)
(double-helix structure of)

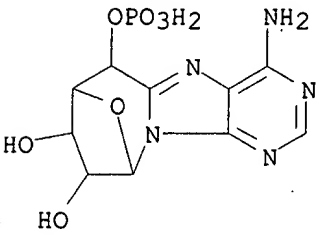
RN 73705-78-9 HCAPLUS
CN .beta.-D-arabino-Uridine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)



L8 ANSWER 42 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:527312 HCAPLUS
DOCUMENT NUMBER: 93:127312
TITLE: NMR studies on the syn-anti dynamic equilibrium in purine nucleosides and nucleotides
AUTHOR(S): Stolarski, Ryszard; Dudycz, Lech; Shugar, David
CORPORATE SOURCE: Inst. Exp. Phys., Univ. Warsaw, Warsaw, PL-02-089, Pol.
SOURCE: Eur. J. Biochem. (1980), 108(1), 111-22
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The syn-anti equil. conformation about the glycosidic bond of purine nucleosides and 5'-nucleotides in different solvent systems was investigated by 1H NMR spectroscopy. Quant. values for the conformer populations were improved, relative to previous results, by a detailed study of, and a resultant derived correction for, the influence of the sugar exocyclic group conformation on the chem. shifts of the sugar ring protons. This was achieved with the aid of nucleosides and nucleotides fixed in the conformations gauche-trans [derivs. of 8,5'-(R)-cycloadenosine nucleosides] and trans-gauche [derivs. of 8,5'-(S)-cyclonucleosides]. The results of 13C NMR confirmed those obtained by 1H NMR. The measured values of the vicinal coupling consts. between H-1' and the C-8 and C-4 atoms were employed to evaluate approx. the glycosidic angles .CHI. of the nucleosides in the conformations syn and anti. A crit. examn. is made of the applicability of relaxation methods, involving anal. of spin-lattice relaxation time of protons (T1) and the Overhauser effect, to det. the conformation of the base about the glycosidic bond; interpretations are provided for the lack of agreement between these methods and those based on chem. shifts in the present study. The foregoing results are also applied to an examn. of the effect of the conformation of the base about the glycosidic bond on the enzymic reactions catalyzed by 5'-nucleotidase and adenosine deaminase.
IT **41036-59-3 41116-92-1**
RL: PRP (Properties)
(NMR of, conformation in relation to)
RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)



RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)

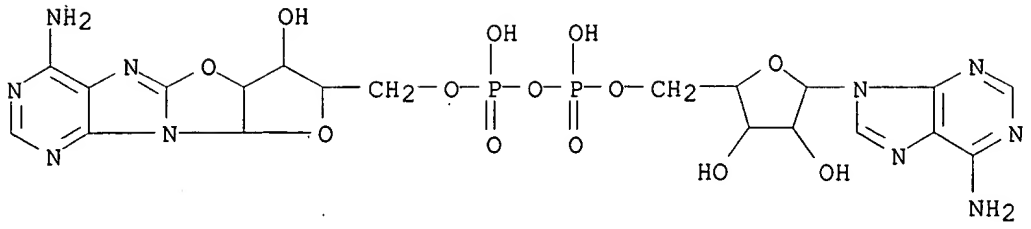


L8 ANSWER 43 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:491436 HCAPLUS
DOCUMENT NUMBER: 93:91436
TITLE: Transfer ribonucleic acids and related compounds. 33. Elongation of oligonucleotides in the 3'-direction with activated mononucleotides and their analogs using RNA ligase
AUTHOR(S): Ohtsuka, E.; Miyake, T.; Nagao, K.; Uemura, H.; Nishikawa, S.; Sugiura, M.; Ikehara, M.
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan
SOURCE: Nucleic Acids Res. (1980), 8(3), 601-10
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English

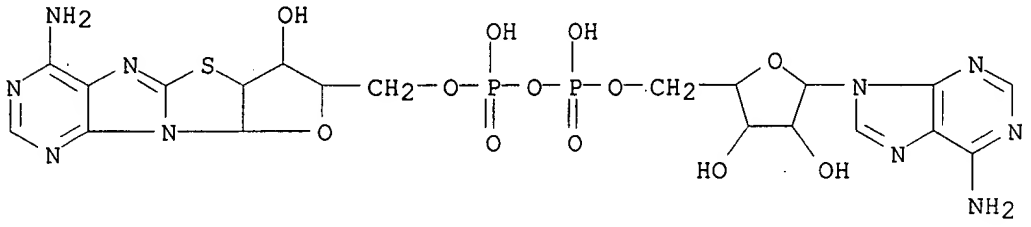
AB P1-Adenosine 5'-p2-2',3'-ethoxymethylidene nucleosides [A(5')ppN(Em)] were prepd. from 4 common nucleosides and used for single addn. of nucleotides to elongate oligonucleotide chains in the 3'-direction in RNA ligase reaction. U-U-C, T-.PSI.-C and A-C-C were used as acceptors. Structural dependence in these acceptors was smaller compared to joining reactions between oligonucleotides. Adenosine analogs: 8-bromo-, 2'-fluoro-, 2'-azido-, 8,2'-O-cyclo-, 8,2'-S-cycloadenosine, arabinosyladenine, and 2'-deoxyadenosine were added to the 3'-end of A-C-C by adenylation chem. followed by joining with RNA ligase. Sym. 5'-pyrophosphates of 8-bromo-, 2'-fluoro-, and 2'-azidoadenosine were not recognized as donor substrates.

IT **73452-44-5 73452-45-6**
RL: RCT (Reactant)
(reaction of, with A-C-C in RNA ligase reaction)

RN 73452-44-5 HCAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), P'-[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]oxazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



RN 73452-45-6 HCAPLUS
CN Adenosine 5'-(trihydrogen diphosphate), P'-[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

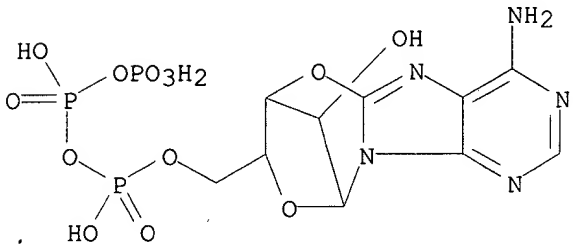


L8 ANSWER 44 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:463716 HCAPLUS
DOCUMENT NUMBER: 93:63716
TITLE: On the chemical communication between the mitochondrial adenine nucleotide carrier and its substrate
AUTHOR(S): Schlimme, Eckhard; Boos, Karl Siegfried; De Groot, Egon Jabbo
CORPORATE SOURCE: Lab. Biol. Chem. Fachber. Naturwiss., Univ. Paderborn, Paderborn, Fed. Rep. Ger.
SOURCE: Mol. Mech. Biol. Recognition, Proc. Aharon Katzir-Katchalsky Conf. (1979), Meeting Date 1978, 443-8. Editor(s): Balaban, Miriam. Elsevier: Amsterdam, Neth.
CODEN: 43GWAZ
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The effect of base, sugar, or phosphate group modification of adenine nucleotides on the carrier protein-mediated translocation mechanism were studied to elucidate the structural requirements of the adenine nucleotide which are essential for recognition by the membrane-bound receptor (carrier-specific binding) and addnl. required to trigger the transfer. Structural modifications of the adenine base were tolerated by the adenine nucleotide carrier, an integral lipoprotein of the inner mitochondrial membrane, with respect to binding and exchange, provided that the electron distributions in the heterocycle, including an unmodified C6-amino group, were retained, i.e. the adenine character of the base remained unchanged. Modification of the phosphate chain had only moderate influence on carrier-specific binding and exchange, provided that the no. of neg. charges in the phosphate chain was unchanged. Modified nucleotide substrates with a conformation equiv. to that of ATP (anti, gauche, gauche) could not be accommodated in the carrier binding site and the

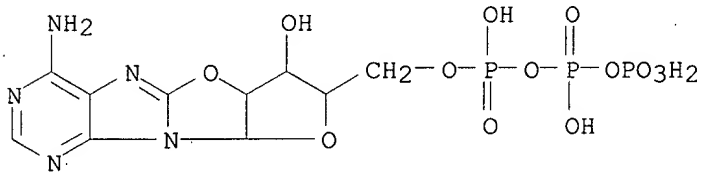
transfer did not occur. The D-configuration of the ribose had to remain unchanged; no inversion of chirality was tolerated by the carrier with the exception of the 3'-hydroxyl group which could be substituted by H. The 2'-hydroxyl group was necessary for the bound nucleotide to trigger the transmembrane adenine nucleotide exchange.

IT **68299-75-2 68299-76-3**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(adenine nucleotide carrier of mitochondria specificity for)

RN 68299-75-2 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]dioxazepino[3,2-e]purin-8-yl)methyl] ester, [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)



RN 68299-76-3 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]oxazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



L8 ANSWER 45 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:408419 HCAPLUS
DOCUMENT NUMBER: 93:8419
TITLE: Polynucleotides. LV. Synthesis and properties of dinucleoside monophosphates derived from adenine 8,2'-S- and uracil 6,2'-O-cyclonucleosides. Further support for the left-handed stacking of oligonucleotides having high-anti base torsion angles
AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi; Shida, Toshio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan
SOURCE: Chem. Pharm. Bull. (1980), 28(1), 189-97
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

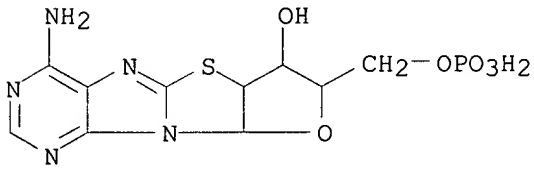
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Dinucleoside monophosphates I and II were synthesized by condensation of suitably protected nucleoside and nucleotide units using dicyclohexylcarbodiimide as a condensing reagent. Examn. of the UV, CD and NMR spectra of these dimers led to the conclusion that, whereas I did not take a stacked conformation, II took a well-stacked conformation, in which the bases were stacked along a left-handed screw axis. The adoption of this conformation could be interpreted in terms of the high base torsion angles in both nucleoside units.

IT **73745-44-5**
RL: RCT (Reactant)
(benzoylation of)
RN 73745-44-5 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, compd. with pyridine (1:2) (9CI) (CA INDEX NAME)

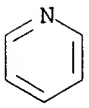
CM 1

CRN 28220-14-6
CMF C10 H12 N5 O6 P S
CDES *




CM 2

CRN 110-86-1
CMF C5 H5 N



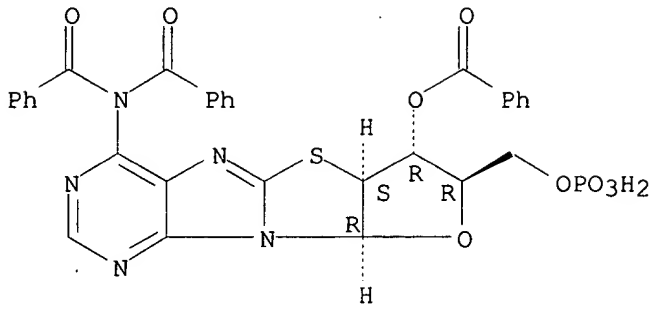

IT **73715-16-9**
RL: RCT (Reactant)
(coupling reaction of, with cyclonucleoside)
RN 73715-16-9 HCAPLUS
CN Benzamide, N-benzoyl-N-[7-(benzoyloxy)-6a,7,8,9a-tetrahydro-8-[(phosphonooxy)methyl]furo[2',3':4,5]thiazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, compd. with pyridine (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 73715-15-8
CMF C31 H24 N5 O9 P S

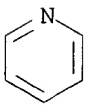
CDES *

Absolute stereochemistry.

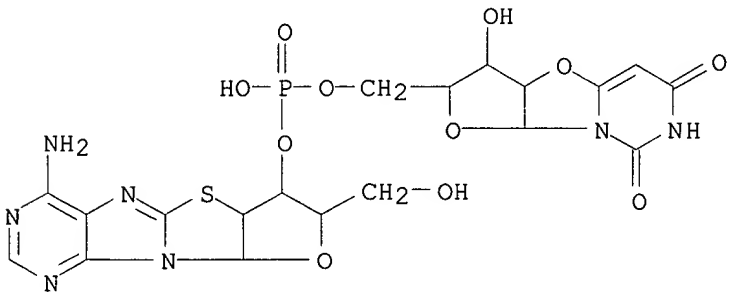


CM 2

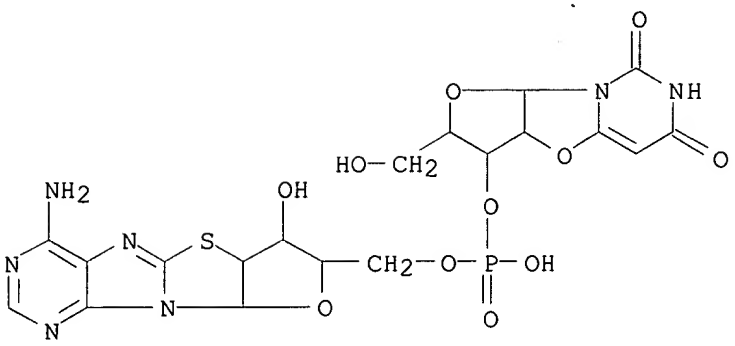
CRN 110-86-1
CMF C5 H5 N



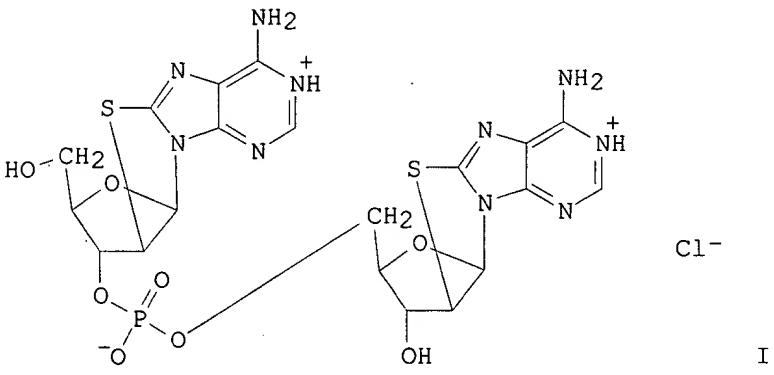
IT **73705-78-9P 73705-79-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and conformation of)
RN 73705-78-9 HCAPLUS
CN .beta.-D-arabino-Uridine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)



RN 73705-79-0 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2',6-anhydro-6-hydroxy-.beta.-D-arabino-uridylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



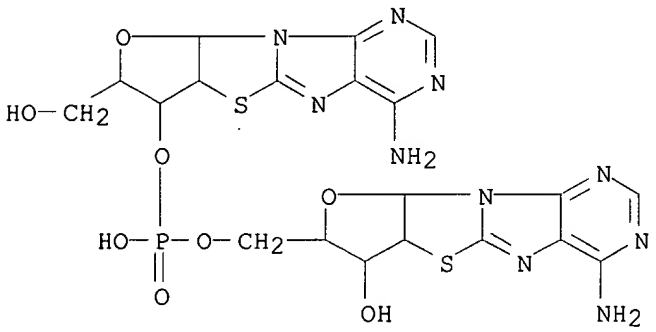
L8 ANSWER 46 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:215683 HCAPLUS
DOCUMENT NUMBER: 92:215683
TITLE: Dinucleoside monophosphate having a high anti conformation: the crystal structure of 8,2'-S-cycloadenylyl-(3'-5')-8,2'-S-cycloadenosine hydrochloride
AUTHOR(S): Fujii, Satoshi; Miura, Reiko; Tomita, Kenichi; Uesugi, Seiichi; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, 565, Japan
SOURCE: Nucleic Acids Symp. Ser. (1979), 6(Symp. Nucleic Acids Chem., 7th), S69-S72
CODEN: NACSD8
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

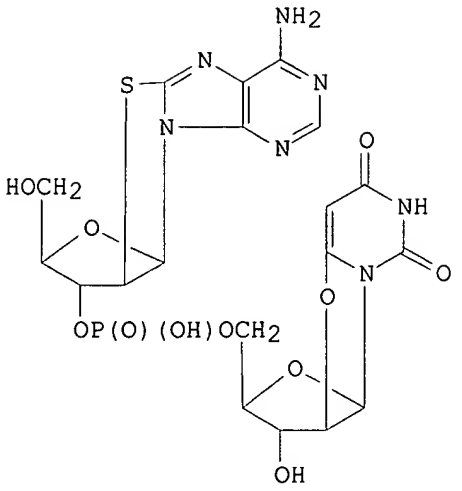
AB The crystal and mol. structure of 8,2'-S-cycloadenylyl-(3'-5')-8,2'-S-cycloadenosine (AspAs) hydrochloride (I) has been detd. by x-ray crystallog. The conformation of 2 independent AspAsmols. found in an asym. unit are almost identical to each other. The torsion angles concerning the sugar-phosphate backbone are different from those in cryst. dinucleoside monophosphates so far detd. by x-rays. Both AspAsmols. are in the sharp bend conformations, i.e. each rotation around P-O bond (.omega.',.omega.) is (g-, t) rather than the preferred (g-, g-) or (g+, g+) conformation. There is no intramol. base stacking or base-pairing but intermol. base stacking was found.

IT **73746-17-5**
RL: PRP (Properties)
(crystal and mol. structure of)
RN 73746-17-5 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L8 ANSWER 47 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:210369 HCAPLUS
DOCUMENT NUMBER: 92:210369
TITLE: The diverse spatial configurations of DNA. Evidence for a vertically stabilized double helix
AUTHOR(S): Sarma, Ramaswamy H.; Dhingra, M. M.; Feldmann, Richard J.
CORPORATE SOURCE: Inst. Biomol. Stereodyn., State Univ. New York, Albany, NY, 12222, USA
SOURCE: Stereodyn. Mol. Syst., Proc. Symp. (1979), 251-64. Editor(s): Sarma, Ramaswamy H. Pergamon: Elmsford, N. Y.
CODEN: 43BTAZ
DOCUMENT TYPE: Conference
LANGUAGE: English
GI



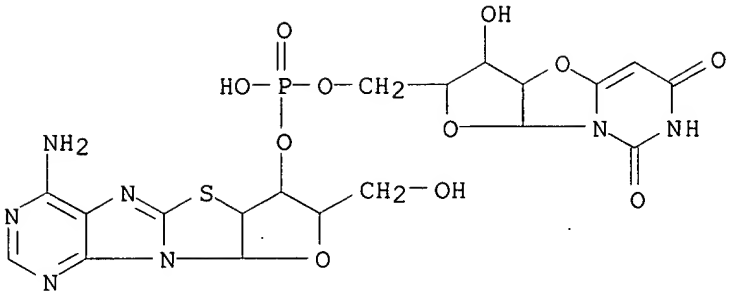
I

AB Evidence for a vertically double-helical DNA configuration was sought by 1H NMR studies of the cyclodinucleotide monophosphate (I) in which the sugar base torsion can adopt a fixed value of .chi.CN .simeq.120.degree. and in which the potential exists for double-helical formation with NMR signals from the base protons being unambiguously assigned. The chem. shift pattern for the self-complementary miniature double helix of I has not been encountered in studies of naturally occurring systems, i.e., ApC, ApU, GpU, CpC and the corresponding deoxyribose systems. Rationalization of the shift of I invoked the interpretation of adenine-adenine overlapping Watson-Crick base-paired double helixes with increasing concns. from 5 to 30 mM. During the helix-coil transition in 2.0M LiCl there was little change in the O-P-O bond of I. The heat of transition and equil. const. for transition were calcd. as 15.7 kcal/mol and 50, resp. Thus, the double helix of I is characterized by strong interstrand adenine-adenine interaction with little intramol. stacking between adenine and uracil of the same strand. Detailed NMR studies of the complementary miniature double helix of ApU implied that if the sugar base torsion angle in the system can adopt a high anti value, it will probably take the vertical double-helical configuration proposed by W. K. Olson (1977). NMR studies of naturally occurring dinucleoside monophosphates have indicated that they are flexible and, thus, capable of conformational pluralism. Comparative data for I and ApU indicated that they adopt different spatial configurations, with ApU having no proclivity for adopting .chi.CN .simeq. 120.degree. and the double-helical array similar to I. The same held for d(pGpC). Thus, the latter 2 self-complementary dinucleoside monophosphates in 2M LiCl have no potential to form double helixes which can be considered of an ordered vertical double helix for the corresponding polynucleotide.

IT **73705-78-9**
RL: BIOL (Biological study)
(vertically stabilized double-helical configuration assumption by, NMR in relation to)

RN 73705-78-9 HCAPLUS

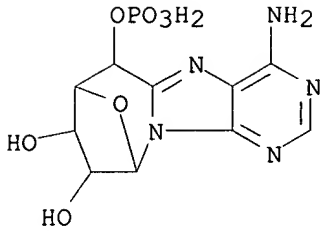
CN .beta.-D-arabino-Uridine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2',6-anhydro-6-hydroxy- (9CI) (CA INDEX NAME)



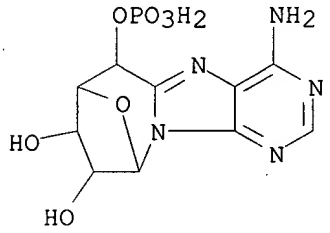
L8 ANSWER 48 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:210355 HCAPLUS
DOCUMENT NUMBER: 92:210355
TITLE: Enzyme-bound conformations of nucleotide substrates. X-ray structure and absolute configuration of 8,5'-cycloadenosine monohydrate
AUTHOR(S): Haromy, Tuli P.; Raleigh, James; Sundaralingam, M.
CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Biochemistry (1980), 19(8), 1718-22
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Irradn. of AMP stereospecifically produces only the C5' epimer of 8,5'-cycloadenosine 5'-monophosphate which is inactive as a substrate for various AMP-utilizing enzymes, whereas the other C5' epimer, from chem. synthesis, is active. The present x-ray study of the nucleoside corresponding to the inactive irradn. product established the abs. configuration to be C(5'S); thus, the active epimer is C(5'R). Crystals of 8,5'-cycloadenosine monohydrate were orthorhombic, space group P212121 (Z = 4), with unit cell dimensions of 4.675(2), 14.605(2), and 17.583(2) .ANG. for a, b, and c, resp. The structure was solved by the multi-soln. technique and refined by the least-squares method to a disagreement index of 0.055 using 1319 intensities. The C3'-C4'-C5'-O5' torsion angle was gauche- (-51.5.degree.) indicating that the active C(5'R) epimer must be trans. Apparently, the trans conformer of AMP is selectively bound to snake venom 5'-nucleotidase and pig muscle AMP kinase and the trans conformer of ADP is bound to rabbit muscle pyruvate kinase. Cyclization constrained the ribose ring to the rare C1'-endo O4'-exo (01T) pucker with pseudorotation parameters P = -72.3.degree. and .tau.m = 47.2.degree.. The fused 6-membered ring C5'-C8-N9-C1'-O4'-C4' assumed a half-chair conformation with the O4' atom puckered. The N6 and N7 atoms of the adenine base formed a pair of hydrogen H-bonds to the O2' and O3' atoms of a symmetry-related ribose. The water of hydration formed a zigzag scheme of H-bonds around a 21 axis.

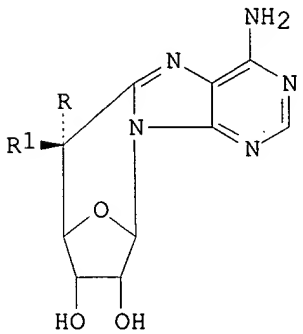
IT **41036-59-3 41116-92-1**
RL: PRP (Properties)
(abs. configuration of)
RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)



RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)



L8 ANSWER 49 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:71728 HCAPLUS
DOCUMENT NUMBER: 92:71728
TITLE: Susceptibility to various enzymes of the carbon-bridged (R) and (S) diastereoisomers of 8,5'-cycloadenosine and their 5'-phosphates
AUTHOR(S): Dudycz, Lech; Shugar, David
CORPORATE SOURCE: Inst. Biochem. Biophys., Acad. Sci., Warsaw, 02-532, Pol.
SOURCE: FEBS Lett. (1979), 107(2), 363-5
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



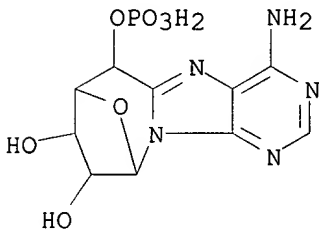
I, R=OH, R1=H
II, R=H, R1=OH

AB The (S) and (R) epimers of 8,5'-cycloadenosine (I and II, resp.) and their

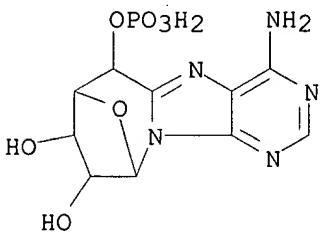
resp. 5'-phosphates were synthesized and their susceptibilities to adenosine deaminase (III) (EC 3.5.4.4), 5'-AMP deaminase (IV) (EC 3.5.4.6), and 5'-nucleotidase (V) (EC 3.1.3.5) were examd. Both I and II were completely resistant to III, I but not II being a weak inhibitor with a Ki of 3 .times. 10-4 M. The 5'-phosphates of I and II were also resistant to IV under conditions where 5'-AMP was completely deaminated in 1 min. With V, I-5'-phosphate showed no reactivity, whereas II-5'-phosphate was slowly (.apprx.0.5% of the rate for 5'-AMP) hydrolyzed. Thus, the formation of the 8,5'-linkage profoundly modifies the nature of the exocyclic group. Both I and II possess a secondary OH and not a primary 5'-OH as in 5'-AMP. This in itself markedly reduces the rate of hydrolysis by V. Hence, the conformation of 5'-AMP interacting with V is defined as anti,gauche-trans.

IT **41036-59-3 41116-92-1**
RL: PRP (Properties)
(reactivity of, with enzymes)

RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)




RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)



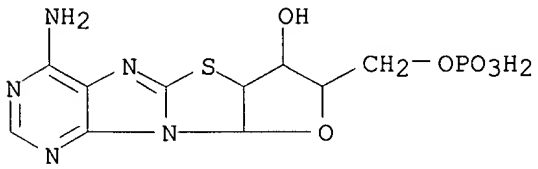

L8 ANSWER 50 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:17911 HCAPLUS
DOCUMENT NUMBER: 92:17911
TITLE: The catalytic site of AMP nucleosidase. Substrate specificity and pH effects with AMP and formycin 5'-phosphate
AUTHOR(S): DeWolf, Walter E., Jr.; Fullin, Frances A.; Schramm, Vern L.
CORPORATE SOURCE: Sch. Med., Temple Univ., Philadelphia, PA, 19140, USA
SOURCE: J. Biol. Chem. (1979), 254(21), 10868-75
CODEN: JBCHA3; ISSN: 0021-9258

DOCUMENT TYPE: Journal
LANGUAGE: English

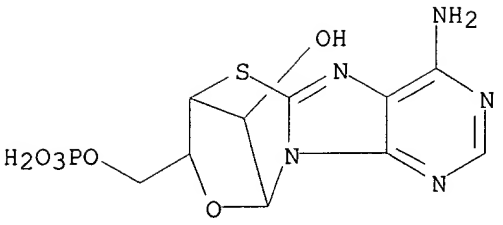
AB AMP nucleosidase from Azobacter vinelandii catalyzed the hydrolysis of the N-glycosidic bond of AMP to give adenine and ribose 5-phosphate. At optimum concns. of the allosteric activator (MgATP), the Km for AMP was 120 .mu.M. Other substrates included 2-aminoAMP, 8-azaAMP, 2'-deoxy-5'-AMP, 3'-deoxy-5'-AMP, and NMN. The Vmax values for these compds. were .ltoreq.10% than the Vmax with AMP as substrate. Most nucleotides and nucleosides were essentially inactive as substrates and were relatively poor inhibitors of the enzyme. This group included IMP, GMP, UMP, CMP, 2'-AMP, 3'-AMP, adenosine, and inosine. The AMP analogs, tubercidin 5'-phosphate, 8-bromoAMP, 8-azidoAMP, 4-aminopyrazolo[3,4-d]pyrimidine-1-ribonucleotide, and 8-spin labeled AMP (8-[[[(2,2,5,5-tetramethyl-1-oxy-3-pyrrolidinyl)carbamoyl]methyl]thio]AMP) were also essentially inactive as substrates, but were good inhibitors of AMP nucleosidase. Thus, the Ki values for these compds. were lower than the Km for AMP. Formycin 5'-phosphate was a linear competitive inhibitor with respect to AMP and exhibited a Ki of 0.043 .mu.M. Thus, the Km/Ki ratio for AMP and formycin 5'-phosphate was >2500. Formycin was a linear competitive inhibitor at low concns. (Ki = 4 .mu.M) but a noncompetitive inhibitor at higher concns. Plots of log Vmax for AMP and pKi for formycin 5'-phosphate as a function of pH values from 6.0 to 9.0 were similar with 2 apparently essential ionizable groups. The pKa values were 6.20 and 8.45 for Vmax and 6.64 and 8.15 for Ki. A plot of log Vmax/Km for AMP was more complex, and suggested that 4 ionizable groups, 2 with a pKa of .apprx.6.60 and 2 with a pKa of .apprx.8.15 were involved. The properties of formycin 5'-phosphate and other AMP analogs with syn-glycosyl torsion angles suggested that the glycosidic torsion angle of AMP changes from the anti toward the syn as substrate binds at the catalytic site. A catalytic mechanism of induced strain on the glycosidic bond, together with electron withdrawal from the purine ring was consistent with the results. A mechanism of N(7) protonation leading to glycosidic bond cleavage was contradicted by the similar pKa values for AMP as substrate and formycin 5'-phosphate as an inhibitor.

IT **28220-14-6 35782-70-8**
RL: BIOL (Biological study)
(AMP nucleosidase response to)

RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)




RN 35782-70-8 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)

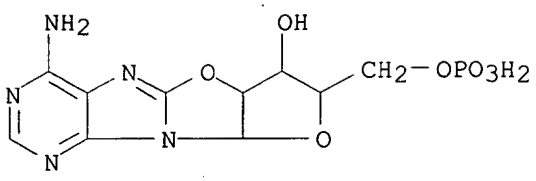


L8 ANSWER 51 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:1735 HCAPLUS
DOCUMENT NUMBER: 92:1735
TITLE: Mitochondrial adenine nucleotide carrier. Investigation of principal structural, steric, and contact requirements for substrate binding and transport by means of ribose-modified substrate analogs
AUTHOR(S): Boos, Karl Siegfried; Schlimme, Eckhard
CORPORATE SOURCE: Lab. Biol. Chem., Univ. Paderborn, Paderborn, D-4790, Fed. Rep. Ger.
SOURCE: Biochemistry (1979), 18(24), 5304-9
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A selected series of 14 ribose-modified adenine nucleotide analogs was prepd. and characterized as the .alpha.-32P- or U-14C-labeled compds. The capacity of rat liver mitochondria for adenine nucleotide carrier-linked (specific) binding and carrier-mediated transfer across the inner mitochondrial membrane as well as the amt. of noncarrier-linked (unspecific) binding of these analogs was detd. at 5.degree. by an inhibitor (atractyloside) stop-method and compared with these values with the natural substrates ADP and ATP. Kinetic data of carrier-specific bound analogs were evaluated from Dixon plots and indicate that these analogs act as competitive inhibitors for mitochondrial ADP and ATP uptake. The findings confirm the distinct substrate specificity of the carrier system. By use of the analogs, an exptl. proof of the 2-step nature of mitochondrial adenine nucleotide translocation, i.e., carrier-specific binding (recognition) and transport, was obtained. Furthermore, the findings provide a detailed description of the basic steric, contact, and structural elements which are prerequisite for carrier-specific binding (A) and addnl. for subsequent transport (B): (A) (1) an anti- or syn-positioned .beta.-N-glycosyl-linked purine base; (2) an S- or N-type sugar pucker; (3) a cis disposition of the C(4')-C(5') bond with respect to the heterocycle; (B) (1) a nonfixed anti-positioned purine base with a N-glycosyl torsion angle of .apprx.-20.degree.; (2) an S-type sugar pucker; (3) a gauche-gauche orientation of the exocyclic C(5')-O(5') group; and (4) a trans-positioned [C(2') ribo] hydroxyl group, which presumably triggers the induction of carrier-mediated transport.

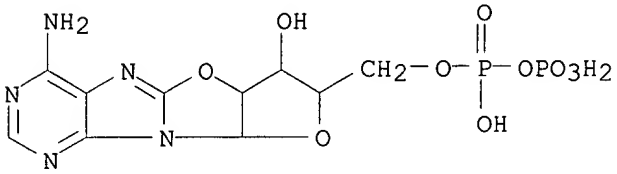
IT **72029-22-2 72029-23-3 72029-24-4**
**72059-47-3 72059-48-4 72074-07-8**
RL: BIOL (Biological study)
(adenine nucleotide carrier of mitochondria interaction with)

RN 72029-22-2 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), monosodium salt, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



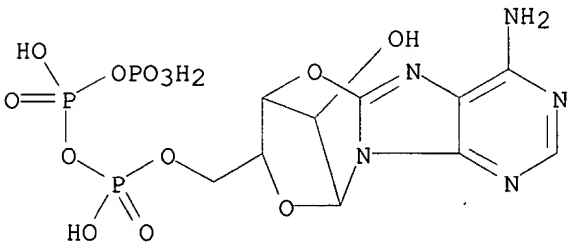
● Na

RN 72029-23-3 HCAPLUS
CN Diphosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]oxazolo[3,2-e]purin-8-yl)methyl] ester, disodium salt, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



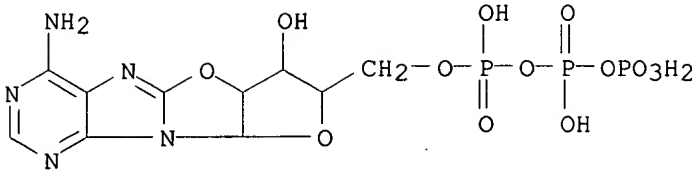
●2 Na

RN 72029-24-4 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]dioxazepino[3,2-e]purin-8-yl)methyl] ester, trisodium salt, [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)



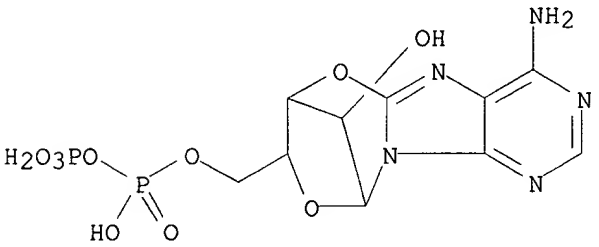
●3 Na

RN 72059-47-3 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]oxazolo[3,2-e]purin-8-yl)methyl] ester, trisodium salt, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



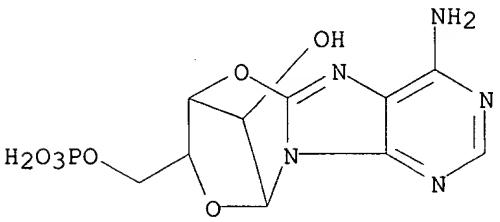
●3 Na

RN 72059-48-4 HCAPLUS
CN Diphosphoric acid, mono[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]dioxazepino[3,2-e]purin-8-yl)methyl] ester, disodium salt, [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)



●2 Na

RN 72074-07-8 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]dioxazepino[3,2-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), monosodium salt, [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)



● Na

L8 ANSWER 52 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:536568 HCAPLUS
DOCUMENT NUMBER: 91:136568

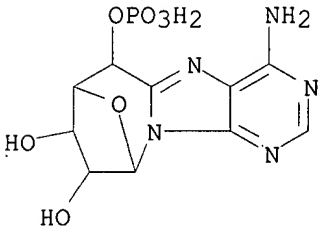
TITLE: Serologic assay of DNA base damage
AUTHOR(S): Lewis, Hazel L.; Ward, John F.
CORPORATE SOURCE: Lab. Nucl. Med. Radiat. Biol., Univ. California, Los Angeles, CA, 90024, USA
SOURCE: ICN-UCLA Symp. Mol. Cell. Biol. (1978), 9(DNA Repair Mech.), 35-8
CODEN: IUSMDJ; ISSN: 0097-9023
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Serol. detns. for hydroxymethyluracil, 8,5'-cycloAMP, and O6-ethylguanosine have been developed using phage neutralization assay and for pyrimidine dimers, using radioimmunoassay. Examples of each system were presented to illustrate the advantages of the serol. approach for the detection and quantitation of DNA damage.

IT **41116-92-1**
RL: ANT (Analyte); ANST (Analytical study)
(detn. of, by immunoassay in DNA base damage anal.)

RN 41116-92-1 HCAPLUS

CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)

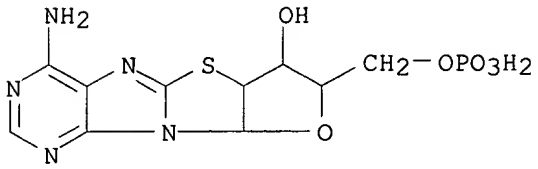



L8 ANSWER 53 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:213560 HCAPLUS
DOCUMENT NUMBER: 90:213560
TITLE: Structural studies of S-cycloadenosine derivatives. I. The crystal and molecular structure of 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine 5'-monophosphate trihydrate (8,2'-S-cyclo 5'-AMP)
AUTHOR(S): Tanaka, Kaori; Fujii, Satoshi; Fujiwara, Takaji; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan
SOURCE: Acta Crystallogr., Sect. B (1979), B35(4), 929-33
CODEN: ACBCAR; ISSN: 0567-7408
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 8.2'-Anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine 5'-monophosphate trihydrate crystd. in the tetragonal system, space group P41212, with a 9.782(1) and c 34.387(5) .ANG.. The structure was solved by the heavy atom method using the intensity data of 1982 independent reflections measured by Zr-filtered Mo K.alpha. radiation and was refined to R = 5.0%. Mols. occur in a high-anti conformation with a glycosidic torsion angle of 118.8.degree.. The ribose conformation is C(4')-endo and the orientation of the C(4')-C(5') bond is gauche-trans. The bases stack along the c axis with interplanar spacing of 3.4 .ANG..

IT **70332-29-5**
RL: PRP (Properties)

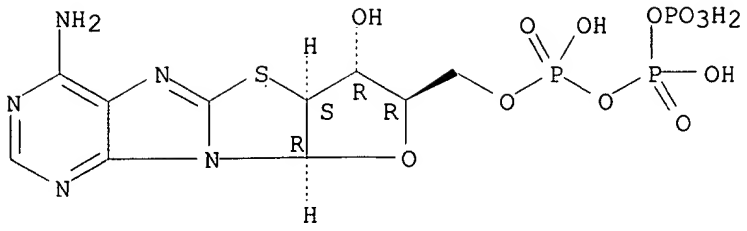
(crystal structure of)
RN 70332-29-5 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), trihydrate, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



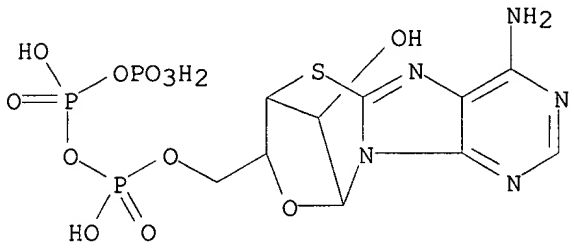
● 3 $H_2O$

L8 ANSWER 54 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:50405 HCAPLUS
DOCUMENT NUMBER: 90:50405
TITLE: Interaction between actomyosin and 8-substituted ATP analogs
AUTHOR(S): Takenaka, Hitoshi; Ikehara, Morio; Tonomura, Yuji
CORPORATE SOURCE: Fac. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1978), 75(9), 4229-33
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Various 8-substituted ATP analogs were synthesized, and their reactions with myosin and actomyosin were studied. The nucleoside triphosphates (NTPs) with an amino group at the 6 position and H at the 8 position and formycin 5'-triphosphate (FTP) were hydrolyzed by myosin very slowly in the presence of Mg2+ and rapidly in the presence of EDTA and K+. In contrast, NTPs with substitution at the 8 position, other than FTP, were readily hydrolyzed by myosin in the presence of Mg2+ but were hardly hydrolyzed in the presence of EDTA and K+. The Km for hydrolysis of 8-substituted NTP by heavy meromyosin was much larger than the dissocn. const. (Kfl) for binding of heavy meromyosin with NTP estd. from the change in tryptophan fluorescence. All the NTPs with no substitution at the 8 position, and FTP, caused an initial PO43- burst, actin activation of myosin NTPase, superpptn. of actomyosin, and myofibrillar contraction. On the other hand, all the 8-substituted NTPs in 3 possible conformations did not cause these phenomena, regardless of the conformation. These results were discussed in relation to the hindrance of rotation about the glycosidic bond accompanying an 8-substitution.
IT **68745-46-0 68745-47-1**
RL: RCT (Reactant)
(reaction of, with myosin ATPase, kinetics of)
RN 68745-46-0 HCAPLUS
CN Triphosphoric acid, P-[[(6aS,7R,8R,9aR)-4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 68745-47-1 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-8-yl)methyl] ester, [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)



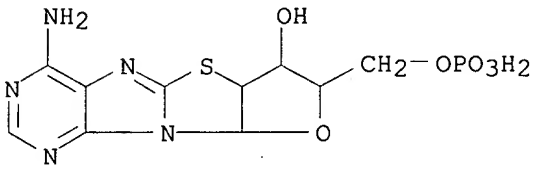
L8 ANSWER 55 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1979:35120 HCAPLUS
DOCUMENT NUMBER: 90:35120
TITLE: Carbon-13 nuclear magnetic resonance spectra of adenine cyclonucleosides and their phosphates. Effects of neighboring groups for elucidation of fine structure of nucleosides and nucleotides
AUTHOR(S): Uesugi, Seiichi; Tanaka, Sumie; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: Eur. J. Biochem. (1978), 90(1), 205-12
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 13C NMR spectra of adenine cyclonucleosides, which have a fixed glycosidic conformation in an anti range, and their isopropylidene and phosphate esters are reported; those of 9-.beta.-D-arabinofuranosyladenine and its 5'-phosphate are also presented. The chem. shifts of the base atoms are affected not only by the bridging atom but also by the position of the bridged sugar C which det. the planarity of the 3rd ring formed by cyclization between the base and the sugar. The effects of the glycosidic conformation on the sugar C chem. shifts are discussed by comparison of the data for 8:5'-cycloadenosines with the data for adenosine and its 8-substituted derivs. The effects of a 2'-O on sugar C chem. shifts were examd. by comparing the data for 2'-deoxyadenosine, arabinosyladenine, and 8:2'-anhydro-8-oxy-9-.beta.-D-arabinofuranosyladenine. The effects of phosphomonoester groups on base and sugar C resonances were examd. and it was noted that these groups cause downfield shifts for C-8 of all cyclonucleotides. Data for the 3':5'-cyclic monophosphate deriv. of 8:2'-anhydro-8-thio-9-.beta.-D-arabinofuranosyladenine suggest that the previous assignments of C-4' and C-3' for nucleoside 3':5'-cyclic monophosphates must be reversed. According to the reversed assignments,

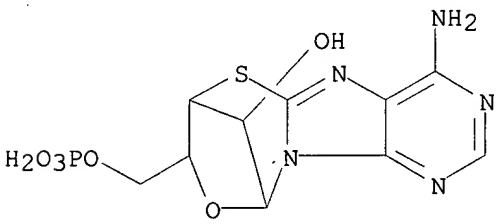
it seems that the C-3' and C-5' show moderate downfield shifts and C-4' shows a marked upfield shift.

IT **28220-14-6 35782-70-8 42735-42-2**
**55652-02-3 56828-07-0 68686-63-5**
RL: PRP (Properties)
(conformation of, NMR in relation to)

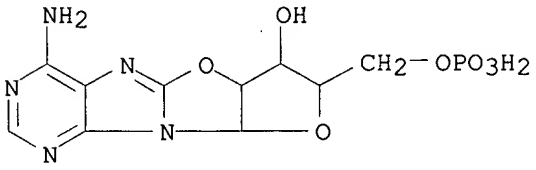
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



RN 35782-70-8 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)

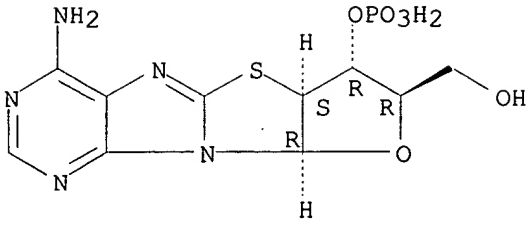


RN 42735-42-2 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



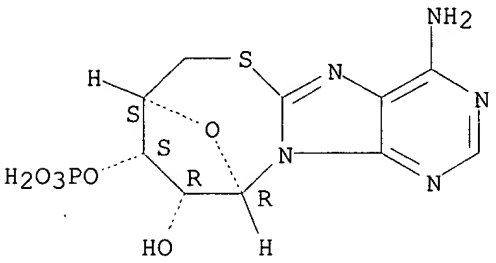
RN 55652-02-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



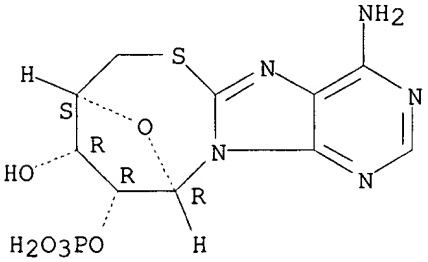
RN 56828-07-0 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 9-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 68686-63-5 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 10-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



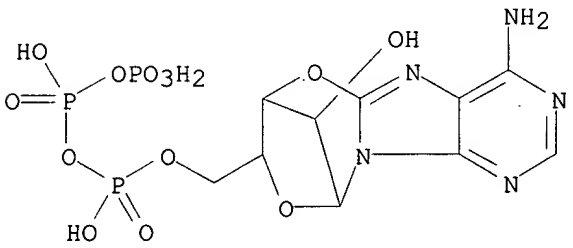
L8 ANSWER 56 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:610523 HCAPLUS
DOCUMENT NUMBER: 89:210523
TITLE: Conformationally restricted adenine nucleotide analogs in mitochondrial adenine nucleotide transport
AUTHOR(S): Boos, Karl Siegfried; Schlimme, Eckhard; Ikehara, Morio
CORPORATE SOURCE: Fachber. Naturwiss., Gesamthochschule Paderborn, Paderborn, Ger.
SOURCE: Z. Naturforsch., C: Biosci. (1978), 33C(7-8), 552-6
CODEN: ZNCBDA; ISSN: 0341-0382

DOCUMENT TYPE: Journal
LANGUAGE: English

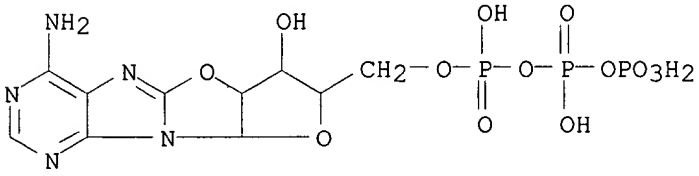
AB The conformationally restricted adenine nucleotide analogs, 8,3'-anhydro-8-oxy-9-(.beta.-D-xylofuranosyl)adenine-5'-O-tri(di)-phosphate and 8,2'-anhydro-8-oxy-9-(.beta.-D-arabinofuranosyl)adenine-5'-O-tri(di)-phosphate, were prepd. chem. as their .alpha.-32P-labeled compds. and compared with syn-structured 8-bromo-AT(D)P in mitochondrial adenine nucleotide translocation. Apparently, the heterocycle-ribose orientation affects the carrier-mediated adenine nucleotide transport very strongly, i.e., a nonfixed adenine heterocycle in the anti region is prerequisite for the bound nucleotide to induce the transfer action of the adenine nucleotide carrier.

IT **68299-75-2 68299-76-3**
RL: BIOL (Biological study)
(adenine nucleotide transport by mitochondria in relation to)

RN 68299-75-2 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]dioxazepino[3,2-e]purin-8-yl)methyl] ester, [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)

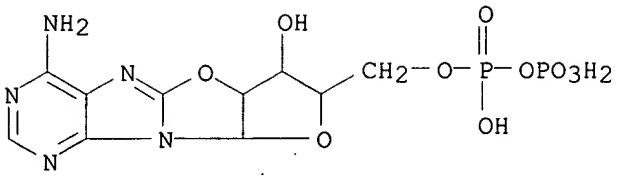


RN 68299-76-3 HCAPLUS
CN Triphosphoric acid, P-[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]oxazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

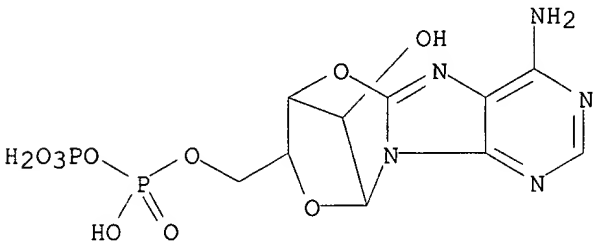


IT **68299-72-9P 68299-77-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 68299-72-9 HCAPLUS
CN Diphosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]oxazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

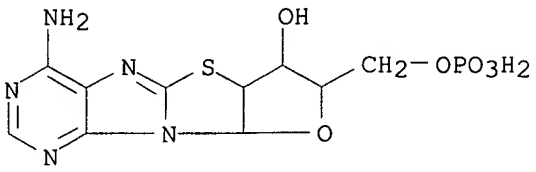


RN 68299-77-4 HCAPLUS
CN Diphosphoric acid, mono[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]dioxazepino[3,2-e]purin-8-yl)methyl] ester, [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)



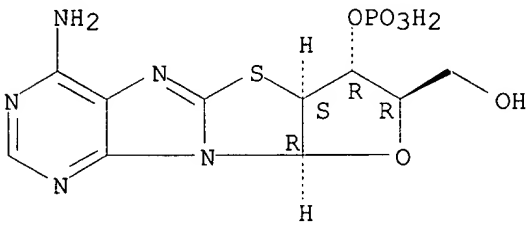
L8 ANSWER 57 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:580275 HCAPLUS
DOCUMENT NUMBER: 89:180275
TITLE: The spatial configuration of a left-handed base stacked dinucleoside monophosphate
AUTHOR(S): Dhingra, M. M.; Sarma, R. H.; Uesugi, S.; Ikehara, M.
CORPORATE SOURCE: Inst. Bimol. Stereodyn., State Univ. New York, Albany, N. Y., USA
SOURCE: J. Am. Chem. Soc. (1978), 100(15), 4669-73
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Detailed 270-MHz NMR studies of the dinucleoside monophosphate of 8,2'-anhydro-8-thio-9-.beta.-D-arabinofuranosyladenine, AspAs, and the component monomers, Asp and pAs, were undertaken. A complete set of NMR parameters was derived for each nucleotidyl unit by simulation-iteration methods. The data indicate that the arabinose ring of the monomers exists as an equil. blend of 2E .dblarw. 3E with bias for 2E pucker. Upon dimerization, the population of 3E pucker increases. In the monomers the C4'-C5' bond shows a distinct preference for gauche-trans and trans-gauche conformations while the conformation about the C5'-O5' bond is gauche'-gauche'. However, in the dimer AspAS, the network contg. C4'-C5' and C5'-O5' bonds prefers the classically stable gauche-gauche and gauche'-gauche' conformation. The C3'-O3' bond exist as a conformation blend of .vphi.1' .simeq. 194.degree. and 286.degree. in which 194.degree. is coupled to 3E sugar pucker and 286.degree. to 2E pucker. The cyclization of the base with the sugar residue introduces constraint on .chi.CN and the magnitude is about 120.degree.. Temp. and dimerization data indicate that despite cyclization a certain amt. of flexibility is accessible to the base-sugar units. A search in the .omega.'.omega. conformation space to account for the dimerization data indicated that .omega.' .simeq. 265 .+-. 5.degree. and .omega. .simeq. 280 .+-. 5.degree.. The nature of the base-base stacking was left-handed in AspAs.

IT **28220-14-6 55652-02-3**
RL: PRP (Properties)
(NMR and conformation of)
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

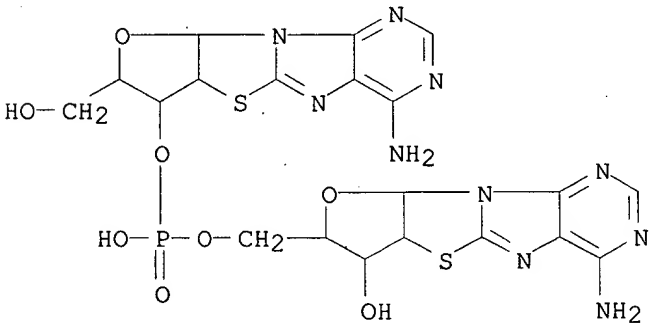


RN 55652-02-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **29617-82-1**
RL: PRP (Properties)
(spatial configuration of)
RN 29617-82-1 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



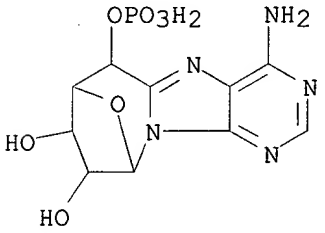
L8 ANSWER 58 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:575566 HCAPLUS
DOCUMENT NUMBER: 89:175566

TITLE: Substrate conformation in 5'-AMP-utilizing enzymes: 8,5'-cycloadenosine 5'-monophosphate
AUTHOR(S): Raleigh, J. A.; Blackburn, B. J.
CORPORATE SOURCE: Whiteshell Nucl. Res. Establ., At. Energy Canada Ltd., Pinawa, Manitoba, Can.
SOURCE: Biochem. Biophys. Res. Commun. (1978), 83(3), 1061-6
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

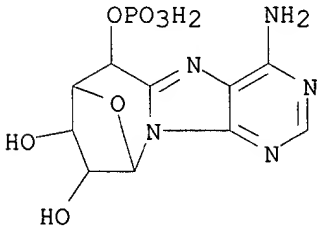
AB One of the two possible C5' epimers of 8,5'-cycloadenosine 5'-monophosphate is a substrate for snake venom 5'-nucleotidase. A stereospecific, radiation chem. synthesis produced one of the epimers in pure form, whose configuration at C5' is established in proton NMR studies. The conformation of 5'-AMP at the active site of 5'-nucleotidase is inferred. This conformation is not in agreement with a previous proposal.

IT **41036-59-3 41116-92-1**
RL: PRP (Properties)
(configuration of, nucleotidase specificity in relation to)

RN 41036-59-3 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)




RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)

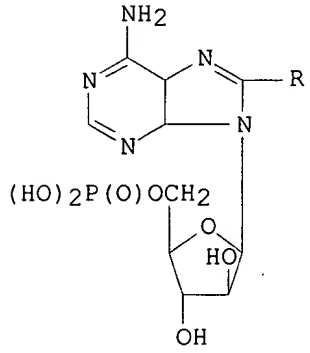



L8 ANSWER 59 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1978:529891 HCAPLUS
DOCUMENT NUMBER: 89:129891
TITLE: 9-(.beta.-D-Arabinofuranosyl)adenine 5'-phosphate
INVENTOR(S): Ikehara, Morio; Shimizu, Fumiharu; Kaneko, Masakatsu
PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan
SOURCE: Japan. Kokai, 5 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 53044591 | A2 | 19780421 | JP 1976-116878 | 19760929 |
| JP 60051480 | B4 | 19851114 | | |

GI



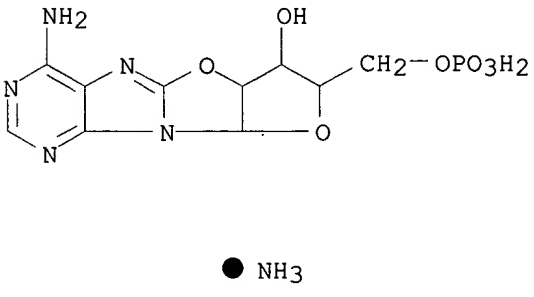
I, R=SH
II, R=H

AB An aq. mixt. of 345 mg 8,2'-O-cycloadenosine 5'-phosphate and 203 mg Bu3N was lyophilized, the resulting ammonium salt (100 mg) was dissolved in pyridine, satd. with H2S, and autoclaved 16 h at 100.degree., concd., and treated with H2O to give an aq. soln. of 8-mercapto-9-(.beta.-D-arabinofuranosyl)adenine 5'-phosphate (I). The aq. soln. contg. 95 mg I was refluxed with Raney Ni 2.5 h to give 31 mg title compd. (II).

IT **67671-01-6**
RL: RCT (Reactant)
(ring cleavage of, with hydrogen sulfide)

RN 67671-01-6 HCAPLUS

CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), monoammonium salt, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



● $NH_3$

L8 ANSWER 60 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:601992 HCAPLUS
DOCUMENT NUMBER: 87:201992
TITLE: Synthesis of 9-(.beta.-D-arabinofuranosyl)adenine

5'-phosphate starting from adenosine 5'-phosphate

AUTHOR(S): Kaneko, Masakatsu; Kimura, Misako; Shimizu, Bunji; Yano, Junichi; Ikehara, Morio

CORPORATE SOURCE: Cent. Res. Lab., Sankyo Co., Ltd., Tokyo, Japan

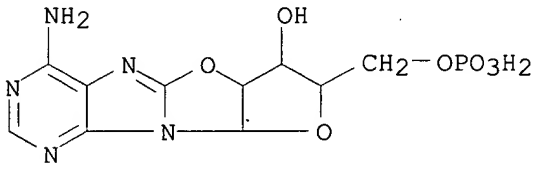
SOURCE: Chem. Pharm. Bull. (1977), 25(8), 1892-8
CODEN: CPBTAL

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 9-(.beta.-D-arabinofuranosyl)adenine 5'-phosphate (I) was obtained from adenosine 5'-phosphate via the novel intermediate 8,2'-O-cycloadenosine 5'-phosphate. Attempted cleavage of this compd. by H2S directly to 8-mercapto deriv. (II) of I failed because of considerable dephosphorylation. N-acylated 8,2'-O-cycloadenosine 5'-phosphate, however, was readily cleaved at the cyclo bond by H2S. Desulfurization of II with Raney Ni gave pure cryst. I.

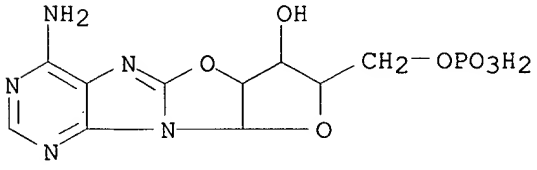
IT **42735-42-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acylation of)
RN 42735-42-2 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



IT **65025-54-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzoylation of)
RN 65025-54-9 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

CM 1

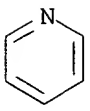
CRN 42735-42-2
CMF C10 H12 N5 O7 P
CDES *



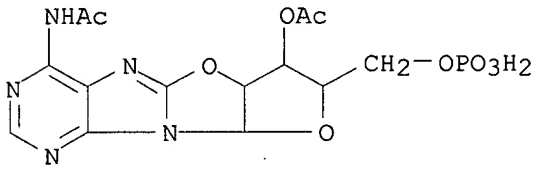
CM 2

CRN 110-86-1

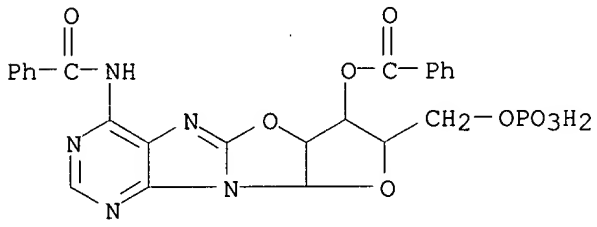
CMF C5 H5 N



IT **52989-04-5P 65030-14-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, and cleavage reaction with hydrogen sulfide)
RN 52989-04-5 HCAPLUS
CN Acetamide, N-[7-(acetyloxy)-6a,7,8,9a-tetrahydro-8-[(phosphonooxy)methyl]furo[2',3':4,5]oxazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



RN 65030-14-0 HCAPLUS
CN Benzamide, N-[7-(benzoyloxy)-6a,7,8,9a-tetrahydro-8-[(phosphonooxy)methyl]furo[2',3':4,5]oxazolo[3,2-e]purin-4-yl]-, [6aR-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



L8 ANSWER 61 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:595736 HCAPLUS
DOCUMENT NUMBER: 87:195736
TITLE: Probing possible left- and right-handed polynucleotide helical conformations from n-h plots. Glycosyl and backbone torsional variation on handedness of helix
AUTHOR(S): Sundaralingam, M.; Yathindra, N.
CORPORATE SOURCE: Coll. Agric. Life Sci., Univ. Wisconsin, Madison, Wis., USA
SOURCE: Int. J. Quantum Chem., Quantum Biol. Symp. (1977), 4(Proc. Int. Symp. Quantum Biol. Quantum Pharmacol., 4th), 285-303
CODEN: IJQBDZ
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The helical parameters n (the no. of nucleotide residues per turn) and h (the residue height along the helical axis) were evaluated for single

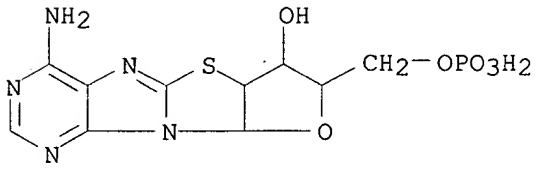
stranded polynucleotide chains and were found to be dependent on the nature of the sugar ring pucker and the nucleotide backbone torsions. The n-h plot reveals that both the familiar right-handed and possible types of left-handed helical conformations fall within the same broad domain, thus conformation transitions from right-handed to left-handed helix and vice versa affect only slightly the backbone torsions. The glycosyl angle apparently suffers the greatest change in the reversal of the helix sense. The normal anti (.chi. .apprx.0-80.degree.) found in right-handed polynucleotides increases to the high anti (.chi. .apprx.125.degree.). These studies indicate that the mol. mechanics of untwisting a helix, leading eventually to a change in helical sense, may involve a combined process of adjusting the glycosyl angle, the pseudorotation phase angle, and the backbone torsions; i.e., helix untwisting perhaps involves synchronous rotations around the glycosyl and backbone bonds. In nucleic acids the left-handed helical conformations are as a rule not favored because the high anti .chi. is not particularly favored. But under certain situations the left-handed base stack and left-handed helical backbone may occur, esp. in short segments around the loop and folded regions of the tertiary structure.

IT **64999-05-9 64999-07-1**
RL: PRP (Properties)
(conformation of, handedness in)

RN 64999-05-9 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, 8-(dihydrogen phosphate), [6aR-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 64999-03-7
CMF C10 H12 N5 O6 P S
CDES *




RN 64999-07-1 HCAPLUS
CN 6H-Furo[2',3':4,5]oxazolo[3,2-c]pyrimidine-6,8(7H)-dione, 2,3,3a,9a-tetrahydro-3-hydroxy-2-[(phosphonooxy)methyl]-, homopolymer, [2R-(2.alpha.,3.beta.,3a.beta.,9a.beta.)]-, complex with [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purine-8-methanol 8-(dihydrogen phosphate) homopolymer (1:1) (9CI) (CA INDEX NAME)

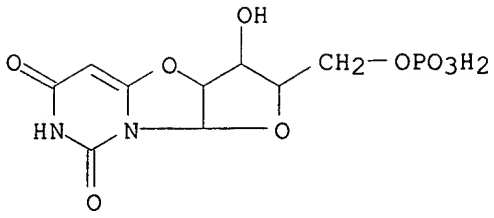
CM 1

CRN 64999-06-0
CMF (C9 H11 N2 O9 P)x
CCI PMS

CM 2

CRN 64999-04-8

CMF C9 H11 N2 O9 P
CDES *

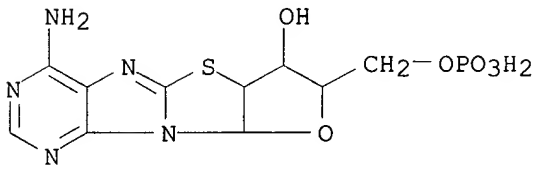


CM 3

CRN 64999-05-9
CMF (C10 H12 N5 O6 P S)x
CCI PMS

CM 4

CRN 64999-03-7
CMF C10 H12 N5 O6 P S
CDES *



=> d ibib abs hitstr 62-94

L8 ANSWER 62 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:468588 HCAPLUS
DOCUMENT NUMBER: 87:68588
TITLE: 9-(.beta.-D-Arabinofuranosyl)adenine-5'-phosphate
INVENTOR(S): Ikehara, Morio; Shimizu, Bunji; Kaneko, Masakatsu
PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan
SOURCE: Japan. Kokai, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 52023094 | A2 | 19770221 | JP 1975-87029 | 19750716 |
| JP 55023280 | B4 | 19800621 | | |

GI For diagram(s), see printed CA Issue.

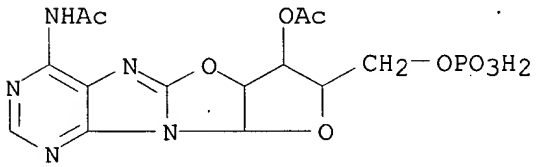
AB Title phosphate I diammonium salt was prepd. from II (R, R1 = aliph. or arom. acyl) by treatment with H2S, removal of the acyl groups, and removal of the SH group (2nd and 3rd steps may be reversed). Thus, H2S was added to 216 mg II monopyridinium salt (R = R1 = Ac) in pyridine over 10 min at -60.degree. and the mixt. autoclaved 11 h at 100.degree. to give 220 mg N6,3'-O-diacetyl-8-mercapto-9-(.beta.-D-arabinofuranosyl)adenine 5'-phosphate monopyridinium salt, 220 mg of which in NH3-satd. MeOH overnight at room temp. gave 160 mg 8-mercapto-9-(.beta.-D-arabinofuranosyl)adenine 5'-phosphate diammonium salt, whch (160 mg) in H2O was refluxed with 0.5 ml Raney-Ni 30 min to give 80 mg I diammonium salt.

IT **63526-46-5**
RL: RCT (Reactant)
(reaction of, with hydrogen sulfide)

RN 63526-46-5 HCAPLUS
CN Acetamide, N-[7-(acetyloxy)-6a,7,8,9a-tetrahydro-8-[(phosphonooxy)methyl]furo[2',3':4,5]oxazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, compd. with pyridine (1:1) (9CI) (CA INDEX NAME)

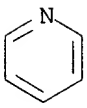
CM 1

CRN 52989-04-5
CMF C14 H16 N5 O9 P
CDES *




CM 2

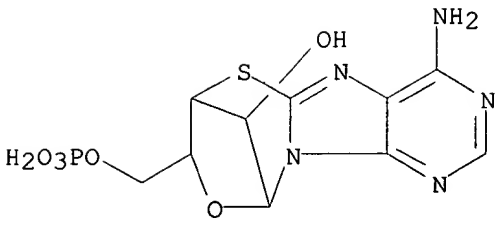
CRN 110-86-1
CMF C5 H5 N



L8 ANSWER 63 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:190401 HCAPLUS
DOCUMENT NUMBER: 86:190401
TITLE: Polynucleotides. 33. Synthesis and properties of the dinucleoside monophosphates containing adenine S-cyclonucleosides and adenosine. Factors determining the stability and handedness of the stacking conformation in a dinucleoside monophosphate
AUTHOR(S): Uesugi, Seiichi; Yano, Junichi; Yano, Emi; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan
SOURCE: J. Am. Chem. Soc. (1977), 99(7), 2313-23
CODEN: JACSAT
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ten dinucleoside monophosphates contg. 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine (As), 8,3'-anhydro-8-mercapto-9-.beta.-D-xylofuranosyladenine (As), 8,5'-anhydro-8-mercapto-9-.beta.-D-ribofuranosyladenine (sA), and adenosine (A) residues were synthesized. AspAs, can take a left-handed stacked conformation at low temp., whereas AspAs and AspAs, the heterodimers of Asand As, may take mainly a left-handed stacked conformation, the stability of which is in-between those of AspAsand AspAs. AspA, AspA, and sApA, the dimers contg. a 5'-linked adenosine and a 3'-linked cycloadenosine residue, take a right-handed stacked conformation. ApAsand ApAs, the dimers contg. a 5'-linked cycloadenosine and a 3'-linked adenosine residue, take a left-handed stacked conformation. SApAs's may take a conformation other than ordinary stacking.
IT **62861-02-3**
RL: RCT (Reactant)
(acetylation of)
RN 62861-02-3 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), compd. with pyridine, [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)

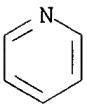
CM 1

CRN 35782-70-8
CMF C10 H12 N5 O6 P S
CDES *

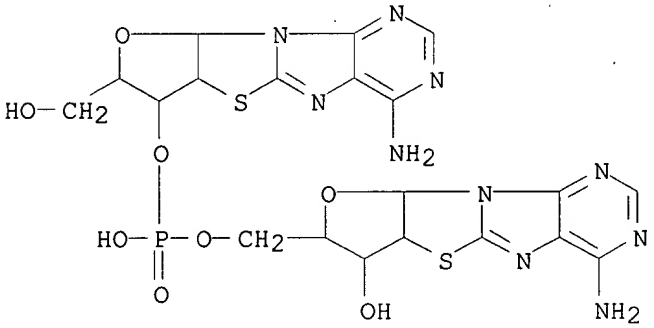


CM 2

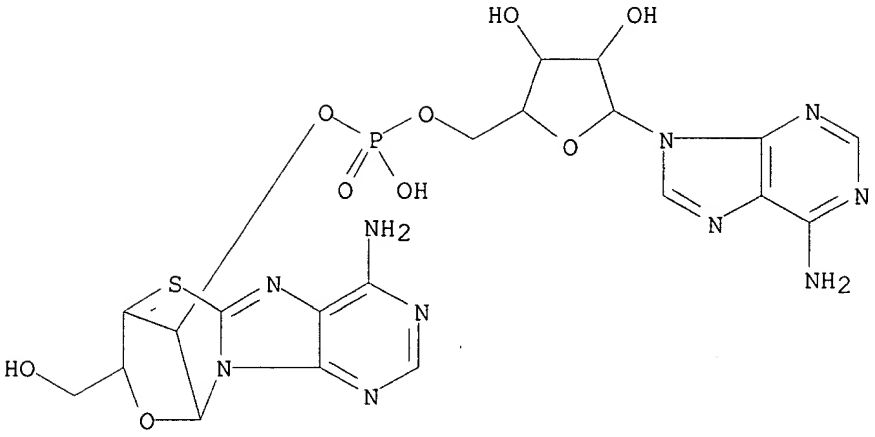
CRN 110-86-1
CMF C5 H5 N



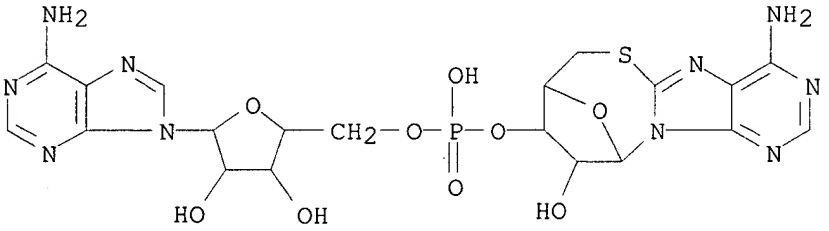
IT **29617-82-1**
RL: RCT (Reactant)
(enzymatic hydrolysis of)
RN 29617-82-1 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



IT **62802-67-9P 62802-69-1P 62850-15-1P**
**62850-16-2P 62850-17-3P 62850-18-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and CD and enzymatic hydrolysis of)
RN 62802-67-9 HCAPLUS
CN 5'-Adenylic acid, mono[4-amino-7,8-dihydro-8-(hydroxymethyl)-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-12-yl] ester, [7S-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)



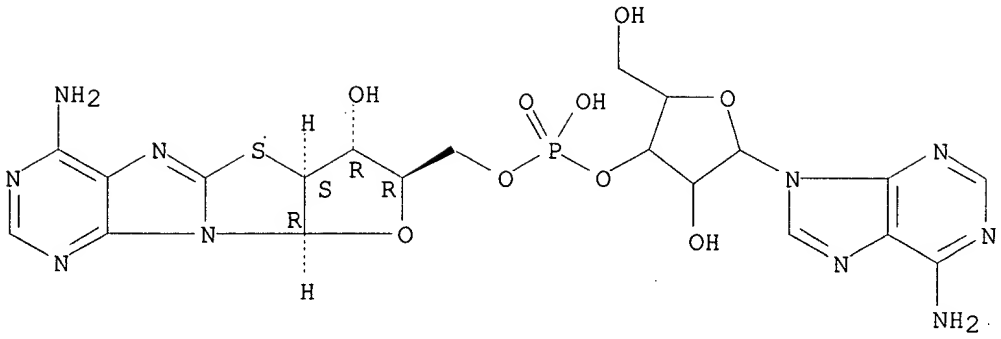
RN 62802-69-1 HCAPLUS
CN 5'-Adenylic acid, mono(4-amino-8,9,10,11-tetrahydro-10-hydroxy-8,11-epoxy-7H-[1,3]thiazocino[3,2-e]purin-9-yl) ester, [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)



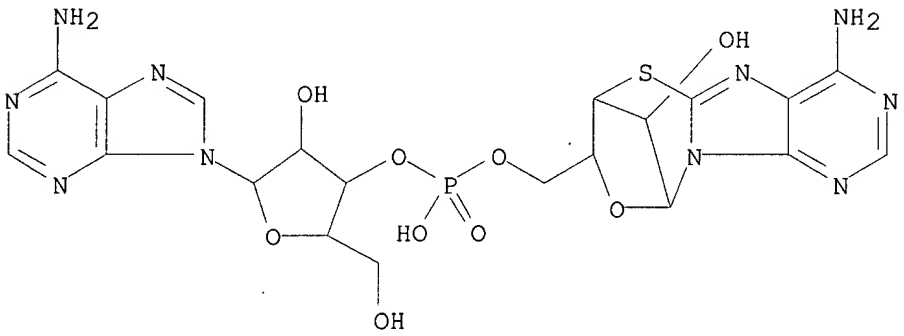
RN 62850-15-1 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-12-[[[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methoxy]hydroxyphosphinyl]oxy]-7,8-dihydro-, [7S-[7.alpha.,8.beta.,10.alpha.,12R*(6aS*,7S*,8R*,9aS*)]]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 62850-16-2 HCAPLUS
CN 3'-Adenylic acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

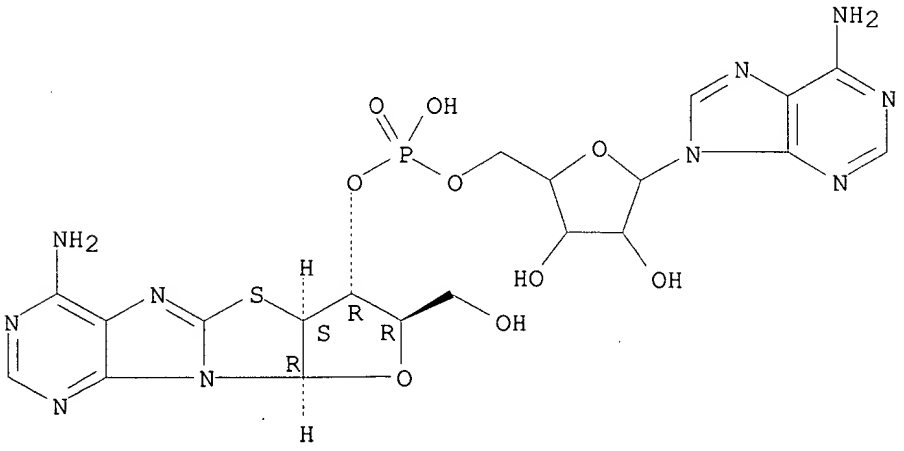


RN 62850-17-3 HCAPLUS
CN 3'-Adenylic acid, mono[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-8-yl)methyl] ester, [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)



RN 62850-18-4 HCAPLUS
CN 5'-Adenylic acid, mono[4-amino-6a,7,8,9a-tetrahydro-8-(hydroxymethyl)furo[2',3':4,5]thiazolo[3,2-e]purin-7-yl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

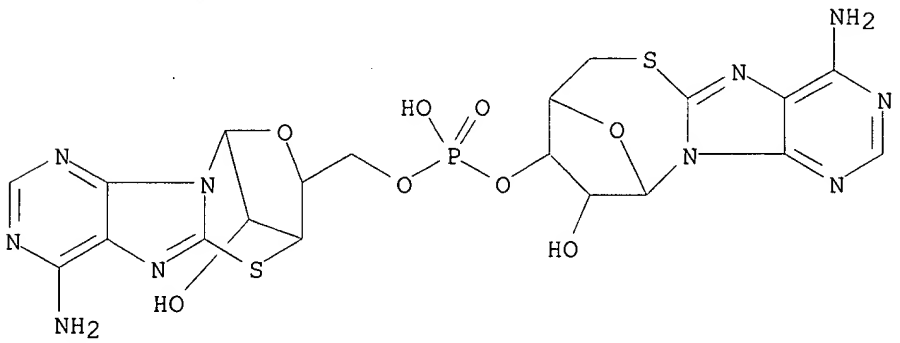


IT **62802-66-8P 62802-68-0P 62850-14-0P**
**62850-19-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymatic hydrolysis of)

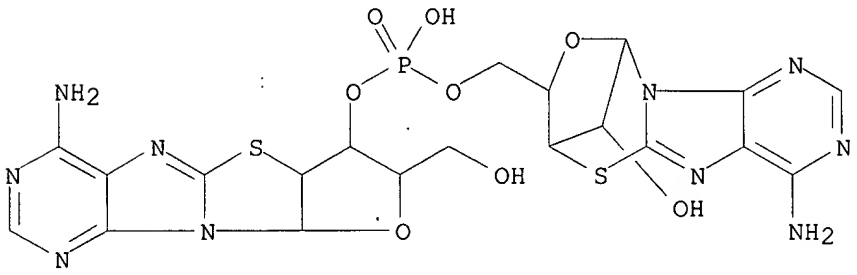
RN 62802-66-8 HCAPLUS
CN Phosphoric acid, mono[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-8-yl)methyl] mono[4-amino-7,8-dihydro-8-(hydroxymethyl)-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-12-yl] ester, [7R-[7.alpha.,8.beta.,10.alpha.,12S*(7S*,8S*,10S*,12R*)]]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

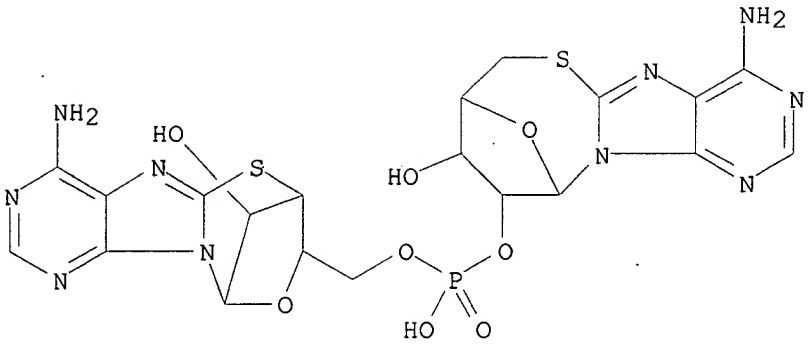
RN 62802-68-0 HCAPLUS
CN Phosphoric acid, mono[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-8-yl)methyl] mono(4-amino-8,9,10,11-tetrahydro-10-hydroxy-8,11-epoxy-7H-[1,3]thiazocino[3,2-e]purin-9-yl) ester, [8S-[8.alpha.,9.beta.(7S*,8S*,10S*,12R*),10.beta.,11.alpha.]]- (9CI) (CA INDEX NAME)



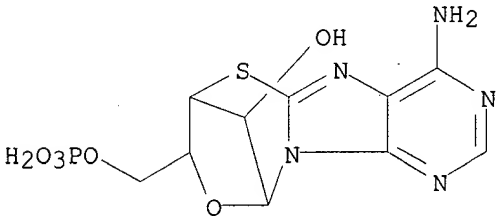
RN 62850-14-0 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-[4-amino-6a,7,8,9a-tetrahydro-8-(hydroxymethyl)furo[2',3':4,5]thiazolo[3,2-e]purin-7-yl hydrogen phosphate], [7R-[7.alpha.,8.beta.(6aR*,7R*,8S*,9aR*),10.alpha.,12S*]]- (9CI) (CA INDEX NAME)



RN 62850-19-5 HCAPLUS
CN Phosphoric acid, mono[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-8-yl)methyl] mono(4-amino-8,9,10,11-tetrahydro-9-hydroxy-8,11-epoxy-7H-[1,3]thiazocino[3,2-e]purin-10-yl) ester, [8S-[8.alpha.,9.beta.(7S*,8S*,10S*,12R*),10.beta.,11.alpha.]]- (9CI) (CA INDEX NAME)

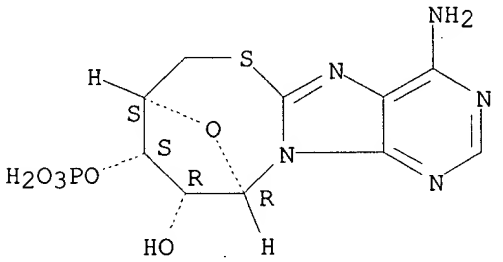


IT **35782-70-8P 56828-07-0P 62802-71-5P**
**62850-20-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35782-70-8 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)

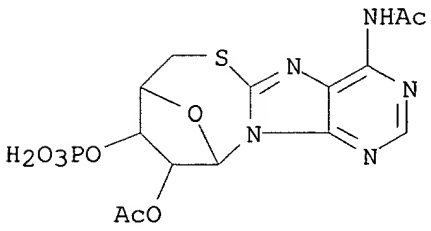


RN 56828-07-0 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 9-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

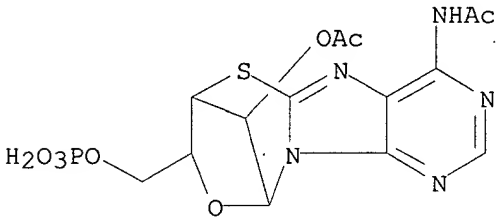
Absolute stereochemistry.



RN 62802-71-5 HCAPLUS
CN Acetamide, N-[10-(acetyloxy)-8,9,10,11-tetrahydro-9-(phosphonooxy)-8,11-epoxy-7H-[1,3]thiazocino[3,2-e]purin-4-yl]-, [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)



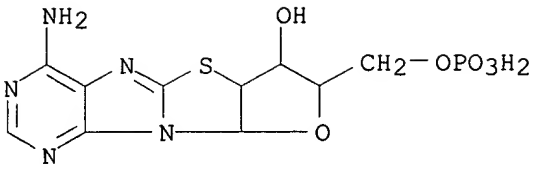

RN 62850-20-8 HCAPLUS
CN Acetamide, N-[12-(acetyloxy)-7,8-dihydro-8-[(phosphonooxy)methyl]-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-4-yl]-, [7S-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)




L8 ANSWER 64 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:106962 HCAPLUS
DOCUMENT NUMBER: 86:106962
TITLE: A semi-empirical potential energy calculation for polynucleotides: the effect of torsion angle .chi. on the helical conformation
AUTHOR(S): Fujii, Satoshi; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan
SOURCE: Nucleic Acids Res., Spec. Publ. (1976), 2(Symp. Nucleic Acids Chem., 4th, 1976), 113-16
CODEN: NARPD6
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The semi-empirical potential energy calcns. of single stranded helical polynucleotide chains showed that the direction of the helical turn and the stereochem. stability of the obtained helical structure were deeply dependent on the glycosyl torsion angles, and the polynucleotides with the high anti conformation around the glycosyl bond could have the left-handed stable helical array with base stacking nearly perpendicular to the helical axis.
IT **52021-41-7**
RL: PRP (Properties)
(effect of torsional angles on conformation of)
RN 52021-41-7 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), homopolymer (9CI) (CA INDEX NAME)

CM 1

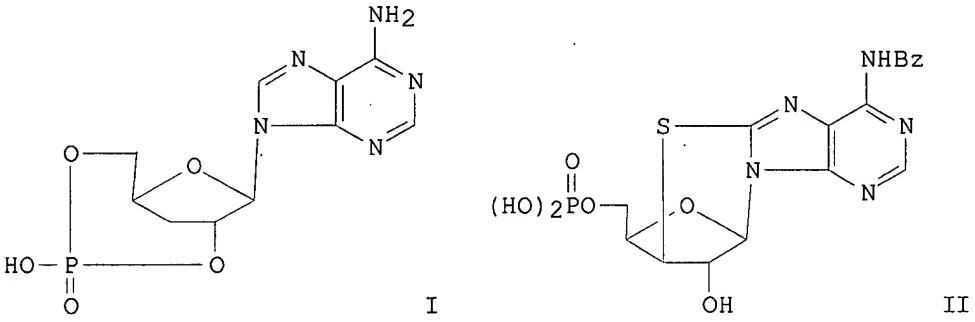
CRN 28220-14-6
CMF C10 H12 N5 O6 P S
CDES *



L8 ANSWER 65 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:73080 HCAPLUS
DOCUMENT NUMBER: 86:73080
TITLE: 3'-Deoxyadenosine 2',5'-cyclic phosphate
INVENTOR(S): Ikehara, Morio; Yano, Junichi
PATENT ASSIGNEE(S): Japan
SOURCE: Japan. Kokai, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 51105093 | A2 | 19760917 | JP 1975-28300 | 19750307 |

GI



I II

AB 3'-Deoxyadenosine 2',5'-cyclic phosphate (I) was prepd. by cyclizing II to its 2',5'-cyclic phosphate with a carbodiimide, followed by debenzoylation and desulfurization. I has antimicrobial and antiviral activities (no data). Thus, II.cntdot.C5H5N and N,N'-dicyclohexyl-4-morpholinocarboxamidine in aq. C5H5N was dehydrated, refluxed with dicyclohexylcarbodiimide, and hydrolyzed with 9N NH3 in MeOH at room temp. for 3 days to give 80% 8,3'-anhydro-8-mercapto-9-.beta.-D-xylofuranosyladenine 2',5'-cyclic phosphate which was refluxed with Raney Ni in H2O for 2 hr to give I ammonium salt.

IT **61848-79-1**
RL: RCT (Reactant)
(cyclodehydration of)

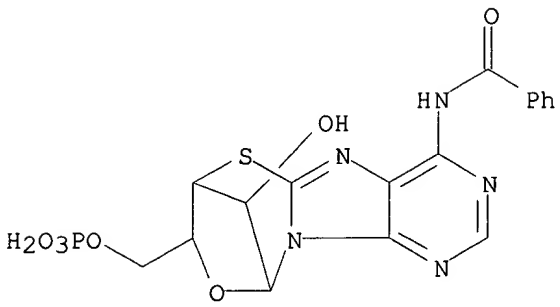
RN 61848-79-1 HCAPLUS

CN Benzamide, N-[7,8-dihydro-12-hydroxy-8-[(phosphonooxy)methyl]-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-4-yl]-, [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]-, compd. with pyridine (1:1) (9CI) (CA

INDEX NAME)

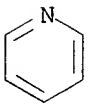
CM 1

CRN 60574-80-3
CMF C17 H16 N5 O7 P S
CDES *



CM 2

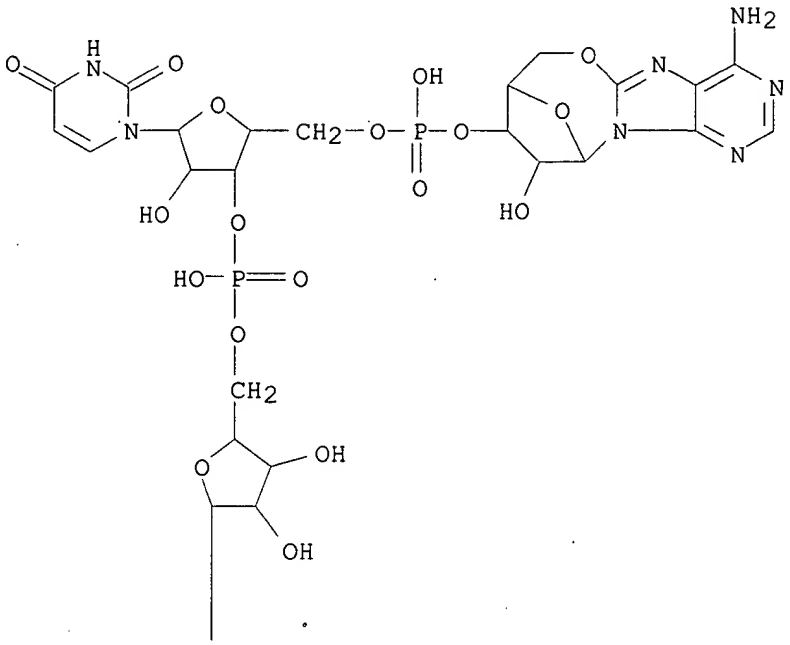
CRN 110-86-1
CMF C5 H5 N



L8 ANSWER 66 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:43959 HCAPLUS
DOCUMENT NUMBER: 86:43959
TITLE: Polynucleotides. XXXIV. Ultraviolet absorption and circular dichroism of ApUpG analogs containing modified adenosine residues
AUTHOR(S): Uesugi, Seiichi; Nagura, Takeo; Ohtsuka, Eiko; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan
SOURCE: Chem. Pharm. Bull. (1976), 24(8), 1884-92
CODEN: CPBTAL
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Uv absorption and CD properties of ApUpG, formycin (F), 8,5'-S-cycloadenosine, 8,2'-S-cycloadenosine, 8,5'-O-cycloadenosine, 8,2'-O-cycloadenosine, 8-bromoadenosine (Br-A) and 8-hydroxyadenosine (HO-A) are reported. S- and O-Cyclonucleosides and F take anti torsion angles while Br-A and HO-A take syn conformation in these trinucleotide analog. All analogs have very weak stacking interaction and tend to form an aggregate at low temp.
IT **52551-06-1 55036-14-1 55048-89-0 55196-42-4**
RL: RCT (Reactant)
(uv spectrum and CD of)

RN 52551-06-1 HCAPLUS
CN Guanosine, 5'-deoxy-5',8-epoxyadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

PAGE 1-A



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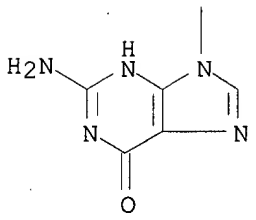
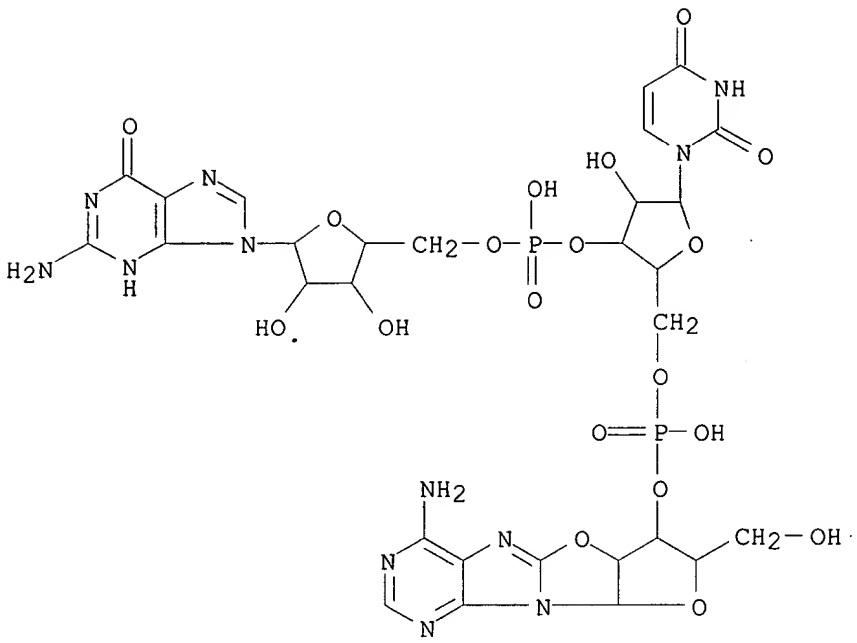
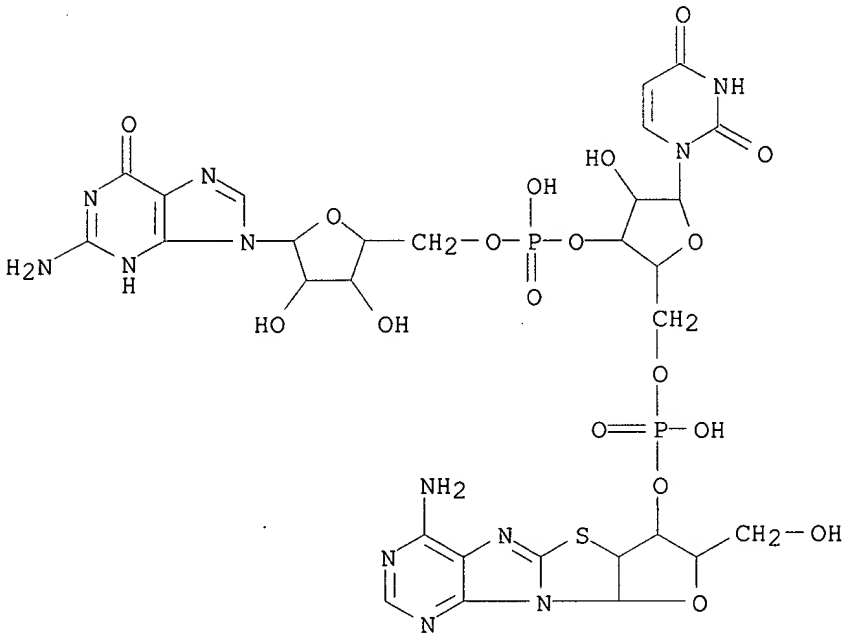


RN 55036-14-1 HCAPLUS
CN Guanosine, 2',8-anhydro-8-hydroxyadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

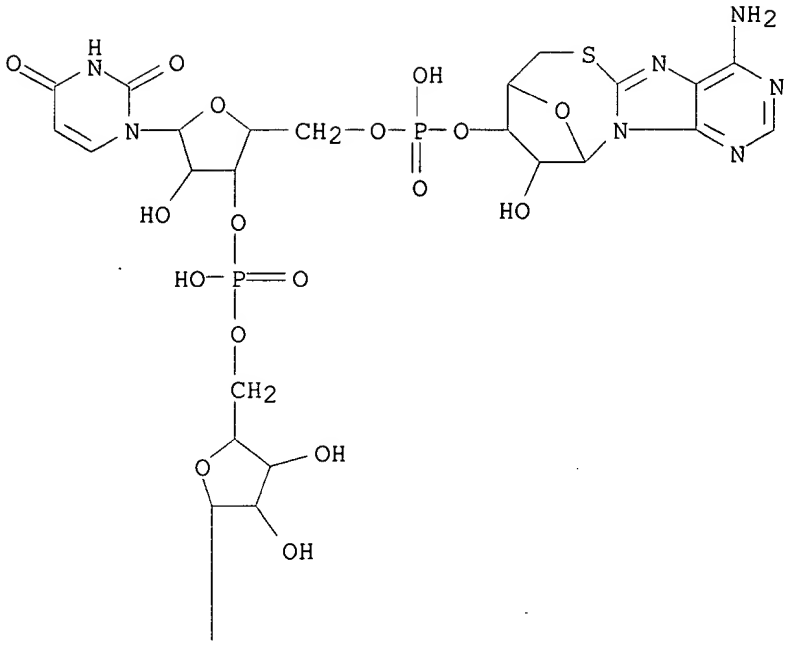


RN 55048-89-0 HCAPLUS
CN Guanosine, 2'-deoxy-2',8-epithioadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

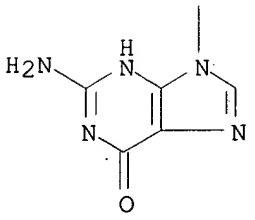


RN 55196-42-4 HCAPLUS
CN Guanosine, 5'-deoxy-5',8-epithioadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L8 ANSWER 67 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1977:16866 HCAPLUS
DOCUMENT NUMBER: 86:16866
TITLE: Conformational analysis of polynucleotides. I. The favorable left-handed helical model for the poly(8,2'-S-cycloadenylic acid) with high anti-conformation
AUTHOR(S): Fujii, Satoshi; Tomita, Kenichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan
SOURCE: Nucleic Acids Res. (1976), 3(8), 1973-84
CODEN: NARHAD
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Energy calcns. show that poly(8,2'-S-cycloadenylic acid) can form left-handed helices owing to the high anti conformation. Two favorable left-handed helices are characterized by axial translation per residue (Z = 4.3 and 3.6 .ANG.) and by rotations per residue (.THETA. = -40.degree.

and -25.degree.). The proposed helical models are stable in aq. soln. and are consistent with the optical property of this compd.

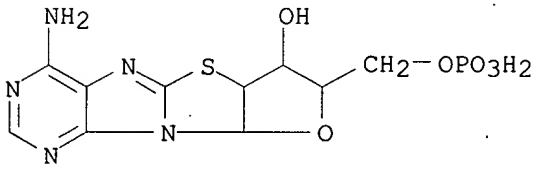
IT **52021-41-7**
RL: PROC (Process)
(conformational anal. of)

RN 52021-41-7 HCAPLUS

CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 28220-14-6
CMF C10 H12 N5 O6 P S
CDES *



L8 ANSWER 68 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:560457 HCAPLUS

DOCUMENT NUMBER: 85:160457

TITLE: Spatial configuration of ordered polynucleotide chains. 3. Polycyclonucleotides

AUTHOR(S): Olson, Wilma K.; Dasika, Rama D.

CORPORATE SOURCE: Douglass Coll., Rutgers State Univ., New Brunswick, N. J., USA

SOURCE: J. Am. Chem. Soc. (1976), 98(17), 5371-80
CODEN: JACSAT

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Approx. details of the spatial configuration of the ordered 8,2'-purine polycyclonucleotide chain in dil. soln. are reported from a combined theor. anal. of chain flexibility and base stacking. Only a fraction of the wide variety of regular polycyclonucleotide helices accommodates the array of stacked bases that characterizes the ordered form of the mol. The bases comprising these stacked helices are arranged almost exclusively in left-handed stacking patterns. The backbone structures to which the stacked polycyclonucleotide bases attach are right-handed helices. The sugar-phosphate units of these polycyclonucleotide helices are identical with backbone conformations deduced in x-ray fiber diffraction analyses of ordered double-stranded polynucleotides. Unlike the bases aligned in planes approx. perpendicular to the long axes of ordered polynucleotide chains, the polycyclonucleotide bases attached to the same backbone frameworks are stacked in planes that approx. parallel the helix axis. This parallel alignment permits the bases of the polycyclonucleotide simultaneously both to exhibit left-handed stacking and to conform to right-handed helical organization.

IT **60828-43-5**
RL: PRP (Properties)
(spatial configuration of)

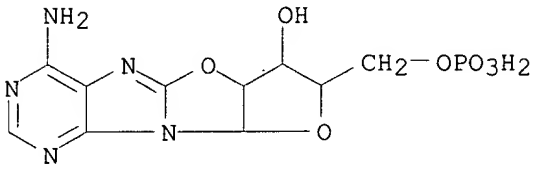
RN 60828-43-5 HCAPLUS

CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-

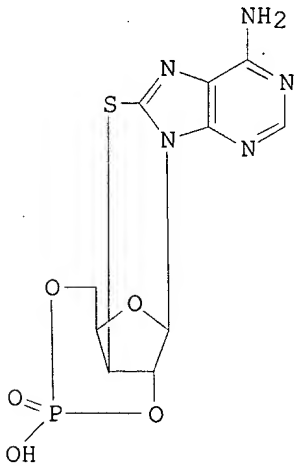
tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 42735-42-2
CMF C10 H12 N5 O7 P
CDES *



L8 ANSWER 69 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:543391 HCAPLUS
DOCUMENT NUMBER: 85:143391
TITLE: Seven-membered cyclic phosphate: synthesis and properties of S-cycloadenosine 2',5'-cyclic phosphate and cordycepin 2',5'-cyclic phosphate. Studies of nucleosides and nucleotides. LXIV. Purine cyclonucleosides. 25
AUTHOR(S): Ikehara, Morio; Yano, Junichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: Nucleic Acids Res. (1974), 1(12), 1783-98
CODEN: NARHAD
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

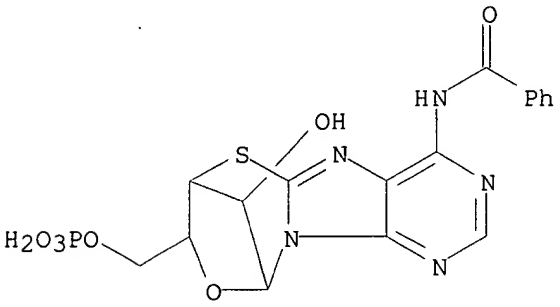


I

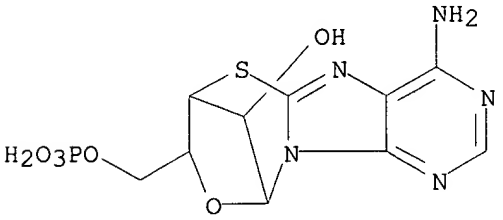
AB The 8,3'-anhydro-8-mercapto-9-.beta.-D-xylofuranosyladenine was phosphorylated with cyanoethyl phosphate and dicyclohexylcarbodiimide (DCC) to 5'-phosphate. After the 6-amino group was benzoylated, the

monophosphate was treated with DCC to give a cyclic phosphate (I), whose structure was elucidated by uv, NMR and CD spectra, as well as enzymatic hydrolyses. Desulfurizing I with Raney Ni gave cordycepin 2',5'-cyclic phosphate.

IT **60574-80-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with morpholinodicyclohexylcarboxamidine)
RN 60574-80-3 HCAPLUS
CN Benzamide, N-[7,8-dihydro-12-hydroxy-8-[(phosphonooxy)methyl]-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-4-yl]-, [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)



IT **35782-70-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 35782-70-8 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)



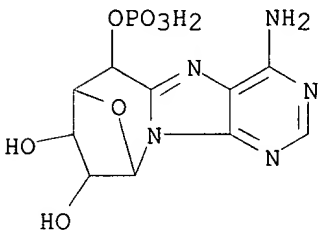
L8 ANSWER 70 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1976:132112 HCAPLUS
DOCUMENT NUMBER: 84:132112
TITLE: Radiation chemistry of nucleotides: 8,5'-cyclonucleotide formation and phosphate release initiated by hydroxyl radial attack on adenosine monophosphates
AUTHOR(S): Raleigh, J. A.; Kremers, W.; Whitehouse, R.
CORPORATE SOURCE: Whiteshell Nucl. Res. Establ., At. Energy Canada Ltd., Pinawa, Manitoba, Can.
SOURCE: Radiat. Res. (1976), 65(3), 414-22
CODEN: RAREAE
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The formation of 8,5'-cycloadenosine 5'-monophosphate (8,5'-cycloAMP) in .gamma.-irradiated solns. of adenosine 5'-monophosphate (5'-AMP), as well as the amt. of phosphates released from solns. of 5'-AMP, adenosine 3'-monophosphate, deoxyadenosine 3'-monophosphate, and deoxyadenosine 5'-monophosphate, was quantified over the pH range 2-10. Maxima for G(8,5'-cycloAMP) occurred at pH 3 and 9 in N- and N2O-satd. soln. O completely inhibited the formation of 8,5'-cycloAMP. Over the pH range 3-10, G(8,5'-cycloAMP) was approx. equal to G(inorg. phosphate) for 5'-AMP. The pH response of both G(inorg. phosphate) and G(8,5'-cycloAMP) appeared to be detd. primarily by the reactivity of the various charged forms of the nucleotides to OH .cntdot. attack.

IT **41116-92-1**
RL: BIOL (Biological study)
(from radiolysis of AMP, hydroxyl in relation to)

RN 41116-92-1 HCAPLUS

CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)




L8 ANSWER 71 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:593629 HCAPLUS

DOCUMENT NUMBER: 83:193629

TITLE: Polynucleotides. XXXII. Further studies on the synthesis of oligonucleotides containing 8,2'-S-cycloadenosine

AUTHOR(S): Ikehara, Morio; Tezuka, Toru

CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan

SOURCE: Nucleic Acids Res. (1975), 2(9), 1539-50
CODEN: NARHAD

DOCUMENT TYPE: Journal

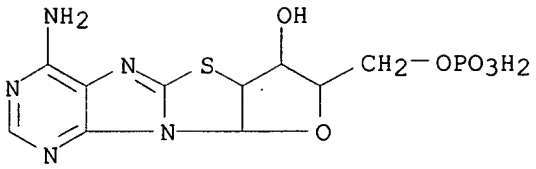
LANGUAGE: English

AB 8,2'-Anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine phosphoryl-(3'-5')-inosine (As pI, As = 8,2'-S-cycloadenosine) was prepd. by condensation of protected 8-mercaptoadenosine 2',3'-cyclic phosphate (I) and 2', 3'-isopropylideneinosine with (PhO)2PPCl. I was polymd. with [(PhO)2P(O)]2O. As oligonucleotides, thus obtained, contained some uncyclized 8-mercaptoadenosine residues and were cleaved at these sites with 0.3N KOH. As 5'-phosphate was prepd. and polymd. with dicyclohexylcarbodiimide to give oligonucleotides with d.p. 2-9.

IT **28220-14-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and benzoylation of)

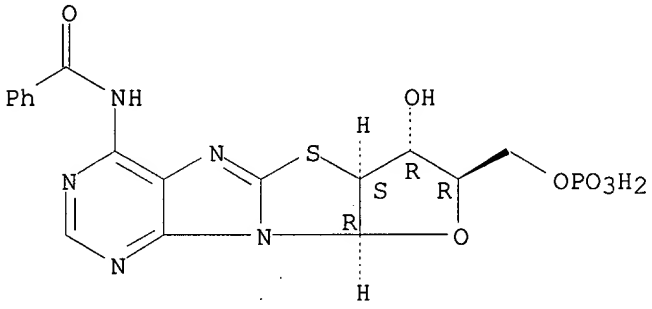
RN 28220-14-6 HCAPLUS

CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



IT **40269-46-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and polymn. of)
RN 40269-46-3 HCAPLUS
CN Benzamide, N-[6a,7,8,9a-tetrahydro-7-hydroxy-8-[(phosphonooxy)methyl]furo[2',3':4,5]thiazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **55132-82-6P 55652-02-3P 57663-70-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 55132-82-6 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-5'-O-phosphono-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)

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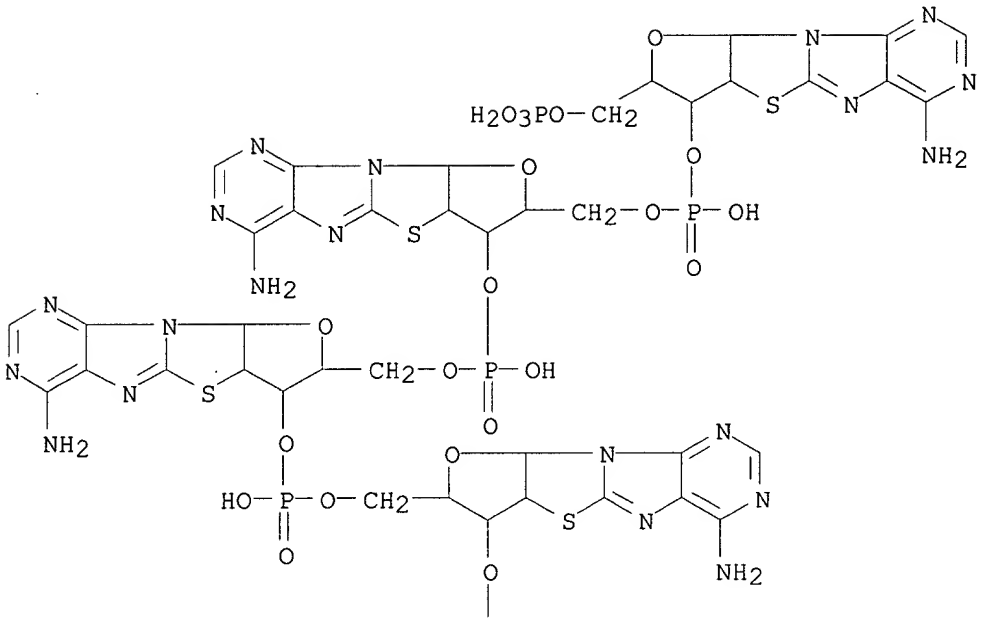

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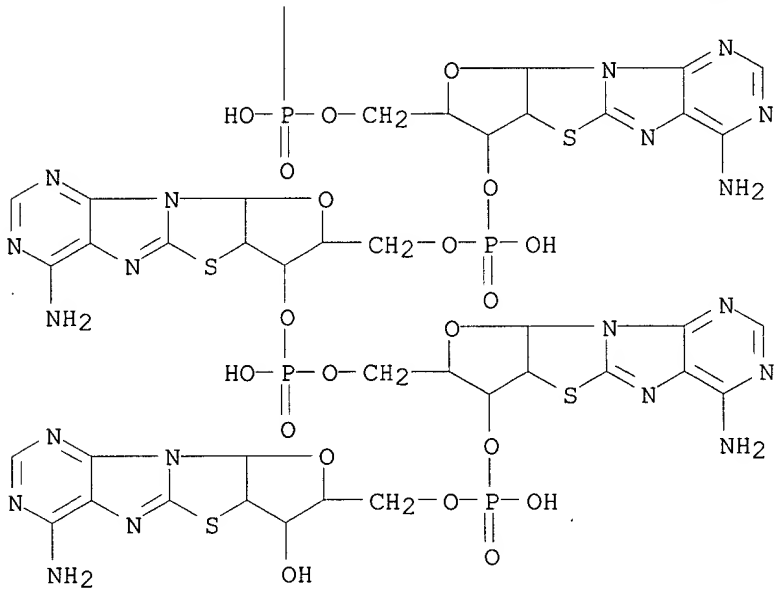
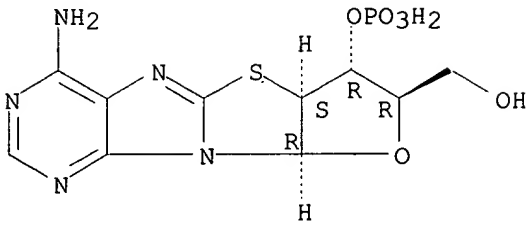
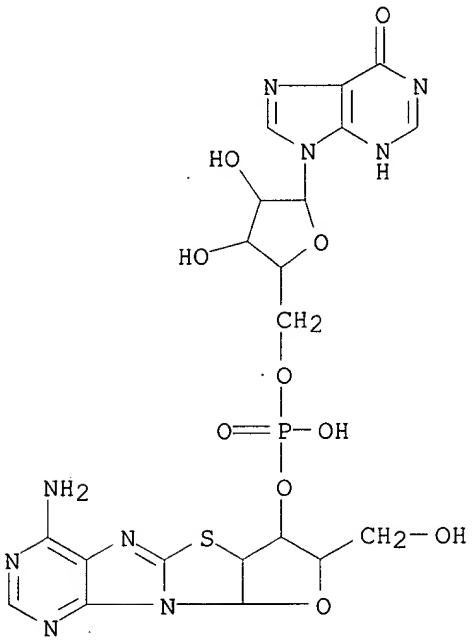


RN 55652-02-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 57663-70-4 HCAPLUS
CN Inosine, 2'-deoxy-2',8-epithioaraadenylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

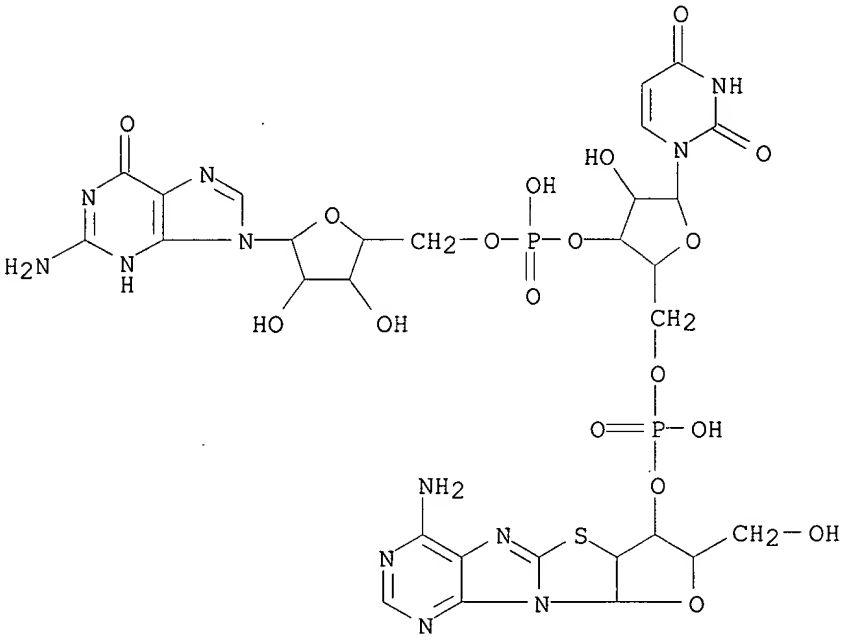


L8 ANSWER 72 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:543205 HCAPLUS
DOCUMENT NUMBER: 83:143205
TITLE: Polynucleotides. XXXI. Synthesis of AUG analogs containing 8,2'-S-cycloadenosine, 8,5'-S-cycloadenosine, 8-bromoadenosine, 8-oxyadenosine, and formycin in the first position of the codon
AUTHOR(S): Ikehara, Morio; Nagura, Takeo; Ohtsuka, Eiko
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Suita, Japan
SOURCE: Nucleic Acids Res. (1975), 2(8), 1345-63
CODEN: NARHAD
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Five AUG analogs having 8,2'-S-cycloadenosine (I), 8,5'-S-cycloadenosine (II), 8-bromoadenosine, 8-oxyadenosine, and formycin (III) in the 1st position of ApUpG were synthesized. The 3'-phosphates of I, II, and III were synthesized. In the case of II, 2',3'-cyclic phosphate was directly

obtained. The 3'-phosphates were properly protected on the 2'-OH and (or) the N6-NH2 group and condensed with 2'-O-benzoyluridylyl(3'-5')-N2, 2',3'-triisobutyrylguanosine to give ApUpG analogs. Paper chromatog., electrophoresis, and uv and CD spectra of these trinucleoside diphosphates are reported.

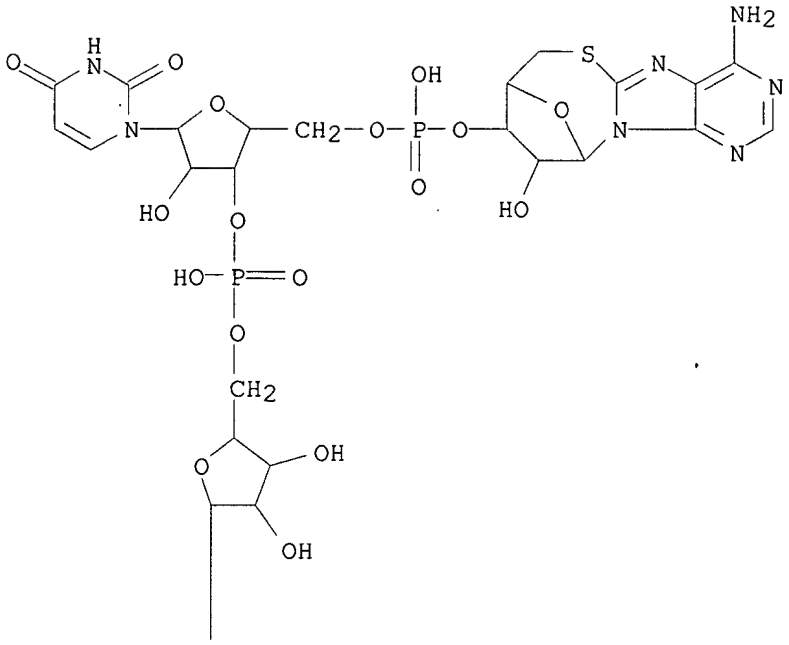
IT **55048-89-0P 55196-42-4P 55652-02-3P**
**56828-00-3P 56828-07-0P 56828-08-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and properties of)

RN 55048-89-0 HCAPLUS
CN Guanosine, 2'-deoxy-2',8-epithioadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)



RN 55196-42-4 HCAPLUS
CN Guanosine, 5'-deoxy-5',8-epithioadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

PAGE 1-A



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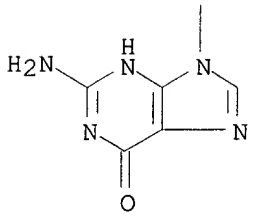
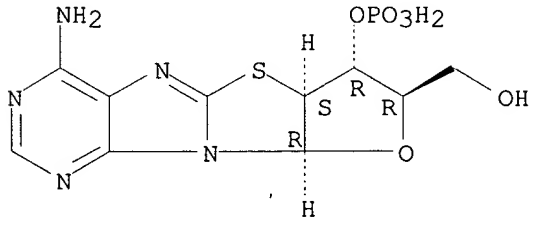


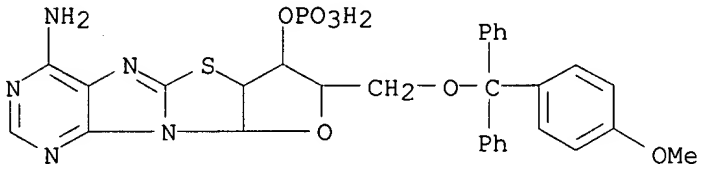
RN 55652-02-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



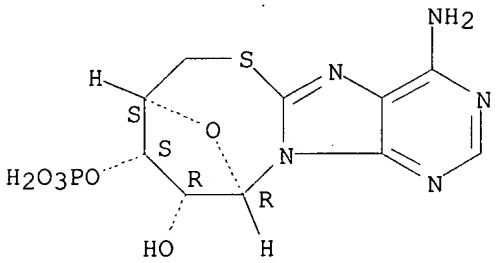
RN 56828-00-3 HCAPLUS

CN Furo[2',3':4,5]thiazolo[3,2-e]purin-7-ol, 4-amino-6a,7,8,9a-tetrahydro-8-[[(4-methoxyphenyl)diphenylmethoxy]methyl]-, dihydrogen phosphate (ester), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

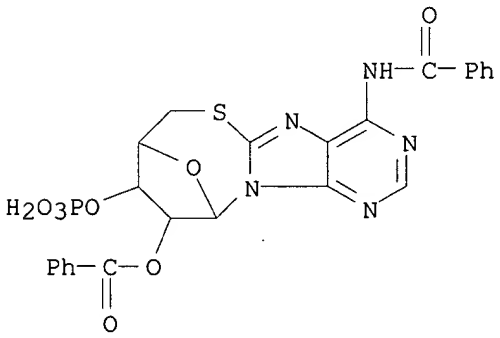


RN 56828-07-0 HCAPLUS
CN 8,11-Epoxy-7H-[1,3]thiazocino[3,2-e]purine-9,10-diol, 4-amino-8,9,10,11-tetrahydro-, 9-(dihydrogen phosphate), [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

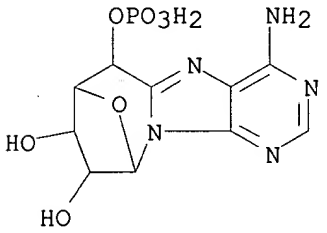


RN 56828-08-1 HCAPLUS
CN Benzamide, N-[10-(benzoyloxy)-8,9,10,11-tetrahydro-9-(phosphonooxy)-8,11-epoxy-7H-[1,3]thiazocino[3,2-e]purin-4-yl]-, [8S-(8.alpha.,9.alpha.,10.alpha.,11.alpha.)]- (9CI) (CA INDEX NAME)



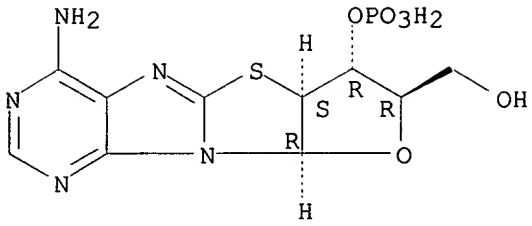
L8 ANSWER 73 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:497796 HCAPLUS
DOCUMENT NUMBER: 83:97796
TITLE: Evidence for reductive radiolytic dephosphorylation in the nucleotide analog 5,5'-cycloadenosine 5'-monophosphate
AUTHOR(S): Raleigh, J. A.; Whitehouse, R.
CORPORATE SOURCE: Med. Biophys. Branch, At. Energy Canada Ltd., Pinawa,

Manitoba, Can.
SOURCE: J. Chem. Soc., Chem. Commun. (1975), (9), 305-6
CODEN: JCCCAT
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Radiolytic phosphate release from the title compd. (I) in H2O was inhibited by N2O, indicating that e-aq. was the species initiating the cleavage. The efficiency of the dephosphorylation coupled with the low reaction rate const. of e-aq. with phosphate ester groups suggested that e-aq. attachment to the purine ring preceded phosphate release.
IT **41116-92-1**
RL: RCT (Reactant)
(radiolytic dephosphorylation of, mechanism of)
RN 41116-92-1 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)



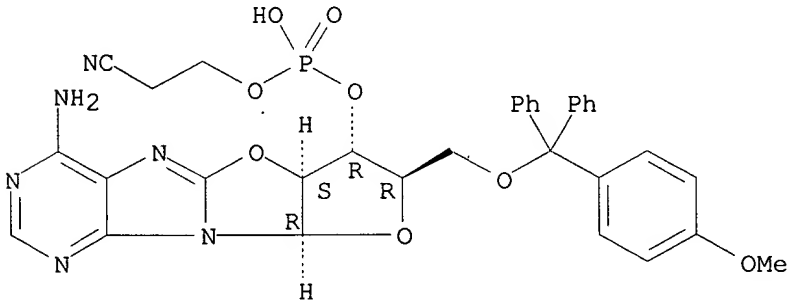

L8 ANSWER 74 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:171337 HCAPLUS
DOCUMENT NUMBER: 82:171337
TITLE: Nucleosides and nucleotides. LVIII. Purine cyclonucleosides. 21. Synthesis of 8,2'-S-cycloadenosine 3'-phosphate from 8-mercaptoadenosine cyclic 2',3'-phosphate using trimethylsilyl chloride
AUTHOR(S): Ikehara, M.; Tezuka, T.
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: J. Carbohyr., Nucleosides, Nucleotides (1974), 1(1), 67-75
CODEN: JCNNAF
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Adenosine 2'-or 3'-monophosphate was converted to the 8-mercapto deriv. with NaSH. Treatment with dicyclohexylcarbodiimide gave 71% 2',3'-cyclic phosphate I. Anhyd. I was treated with Me3SiCl to give 75% II.
IT **55652-02-3**
RL: RCT (Reactant)
(dephosphorylation of)
RN 55652-02-3 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-(phosphonooxy)-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

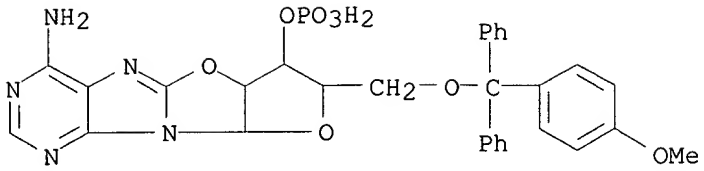


L8 ANSWER 75 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:140429 HCAPLUS
DOCUMENT NUMBER: 82:140429
TITLE: Polynucleotides. XXVI. Synthesis of an AUG [adenylyl-(3'-5')-aridylyl-(3'.far.5')-guanosine] analog, 8,2'-anhydro-8-oxy-9-.beta.-D-arabinofuranosyladenine phosphoryl-(3'-5')-uridylyl-(3'-5')-guanosine
AUTHOR(S): Ikehara, Morio; Nagura, Takeo; Ohtsuka, Eiko
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: Chem. Pharm. Bull. (1974), 22(11), 2578-86
CODEN: CPBTAL
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The title AUG analog I was prepd. in 4.1% yield from 2'-O-(2,4,6-triisopropylbenzenesulfonyl)-8-bromoadenosine in 6 steps. I showed hypochromicity of 7.3% at 257 nm, the CD spectra taken at 0.degree. and 20.degree. showed that this trinucleotide exists in a freely rotatable, unstacked form at both these temps.
IT **55036-11-8P 55036-12-9P 55036-14-1P**
**55036-17-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 55036-11-8 HCAPLUS
CN Phosphoric acid, mono[4-amino-6a,7,8,9a-tetrahydro-8-[[(4-methoxyphenyl)diphenylmethoxy]methyl]furo[2',3':4,5]oxazolo[3,2-e]purin-7-yl]mono(2-cyanoethyl) ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

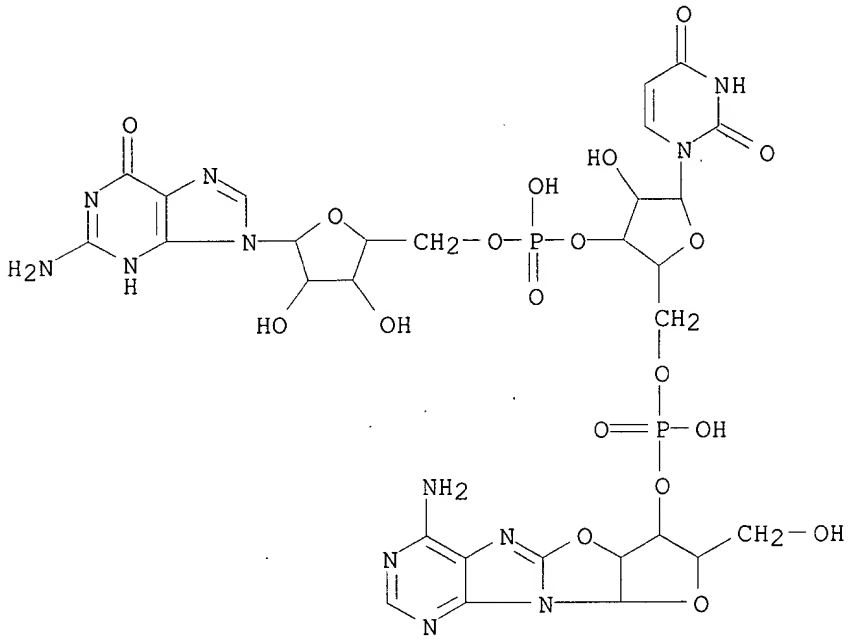
Absolute stereochemistry.



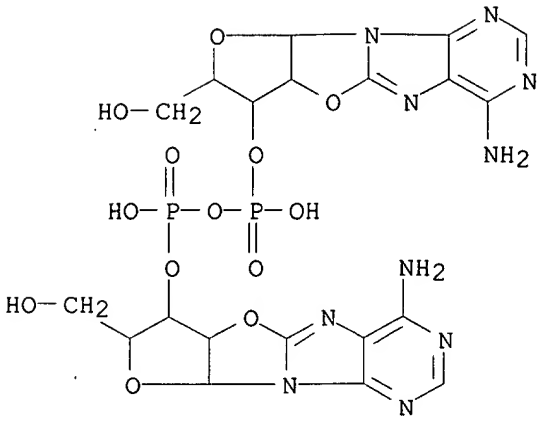
RN 55036-12-9 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purin-7-ol, 4-amino-6a,7,8,9a-tetrahydro-8-[[(4-methoxyphenyl)diphenylmethoxy]methyl]-, dihydrogen phosphate (ester), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



RN 55036-14-1 HCAPLUS
CN Guanosine, 2',8-anhydro-8-hydroxyadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)



RN 55036-17-4 HCAPLUS
CN Diphosphoric acid, P,P'-bis[4-amino-6a,7,8,9a-tetrahydro-8-(hydroxymethyl)furo[2',3':4,5]oxazolo[3,2-e]purin-7-yl] ester, [6aS-[6a.alpha.,7.alpha.(6aR*,7S*,8S*,9aS*),8.beta.,9a.alpha.]]- (9CI) (CA INDEX NAME)



L8 ANSWER 76 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:134186 HCAPLUS
DOCUMENT NUMBER: 82:134186
TITLE: Polynucleotides. XXVIII. Stimulation of the binding of aminoacyl-tRNA to ribosomes by tri- and polynucleotide analogs
AUTHOR(S): Ohtsuka, Eiko; Nagura, Takeo; Shimokawa, Kikuo; Nishikawa, Satoshi; Ikehara, Morio
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Biochim. Biophys. Acta (1975), 383(3), 236-41
CODEN: BBACAQ
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Messenger activity of synthetic tri- and polynucleotide analogs was studied by binding of 14C-labeled aminoacyl-tRNAs to ribosomes in the presence of the analogs. Synthetic messengers used were: poly(A) analogs in which adenosine was replaced by tubercidin, 3-deazaadenosine, 1-deazaadenosine, and 2-methyladenosine; copolymers of adenosine and aristeromycin; cyclic triadenylate; the heptanucleotide of 6,2'-O-cyclouridine; the pentanucleotide of 8,2'-S-cycloadenosine; and ApUpG analogs in which adenosine was replaced by 8,2'-O- and S-cycloadenosine, 8,5'-O- and S-cycloadenosine, 8-oxyadenosine, 8-bromoadenosine, and formycin. Among these oligo- and polynucleotides, analogs which contained nucleotides of anti conformation having appropriate bases for Watson-Crick type H bonding stimulated the binding of corresponding tRNAs to ribosomes.

IT **52551-06-1 55036-14-1 55048-68-5**
**55048-89-0 55196-42-4**
RL: BIOL (Biological study)
(aminoacyl-tRNA-ribosome binding in relation to)

RN 52551-06-1 HCAPLUS
CN Guanosine, 5'-deoxy-5',8-epoxyadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

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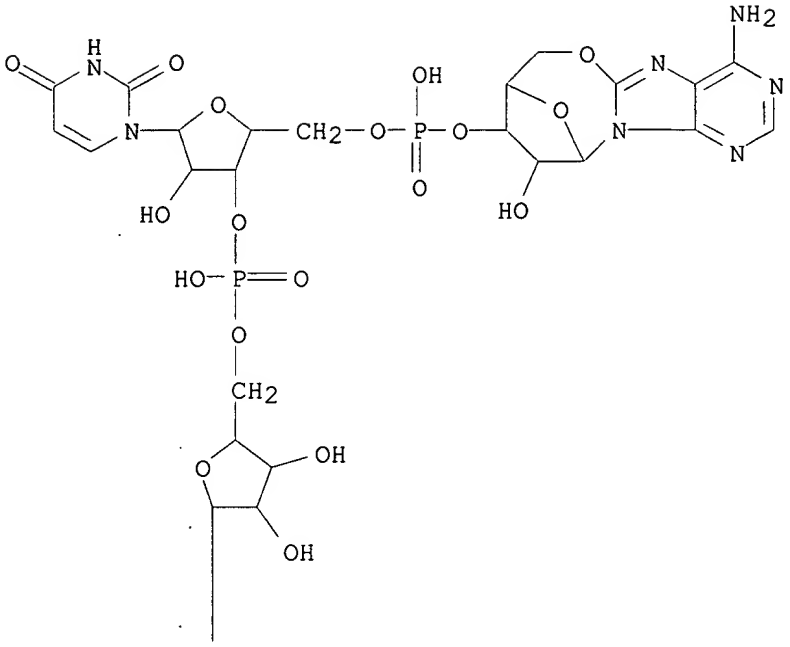
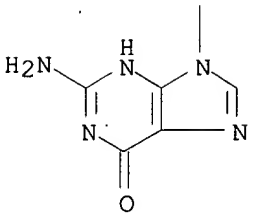
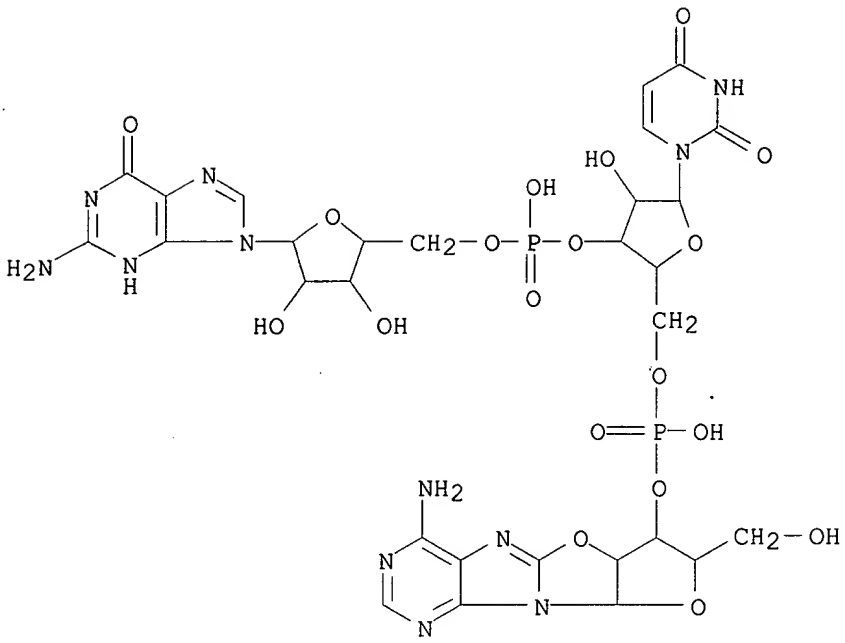


PAGE 2-A



RN 55036-14-1 HCAPLUS
CN Guanosine, 2',8-anhydro-8-hydroxyadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)



RN 55048-68-5 HCAPLUS
CN .beta.-D-arabino-3'-Adenylic acid, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)

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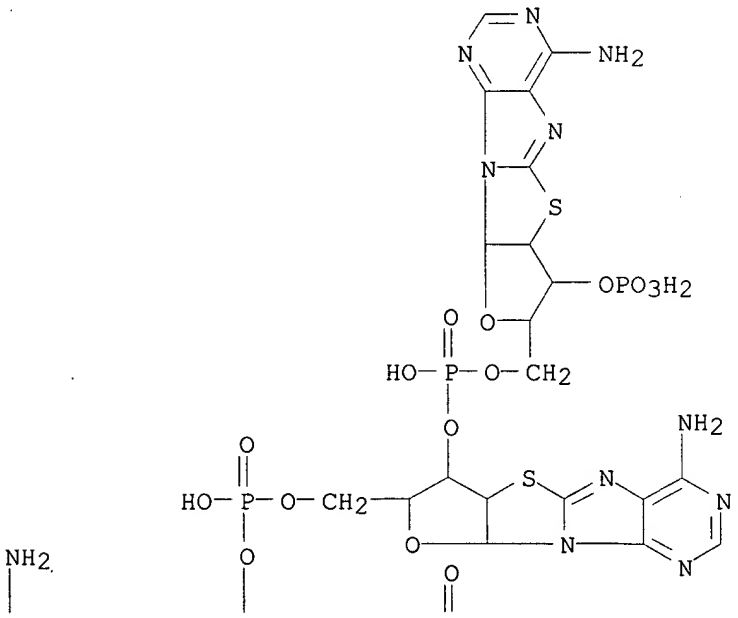
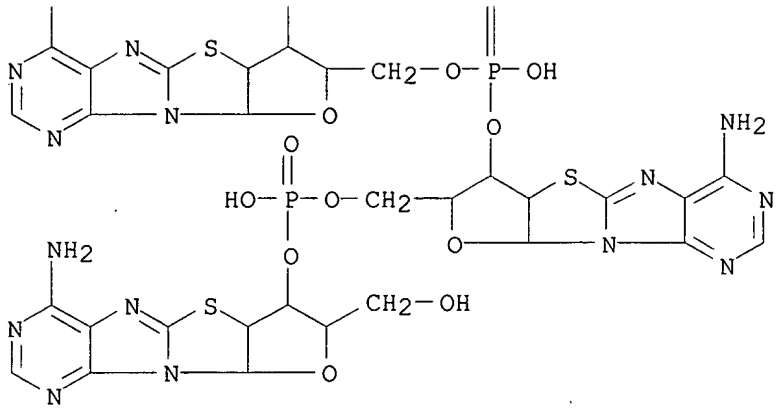
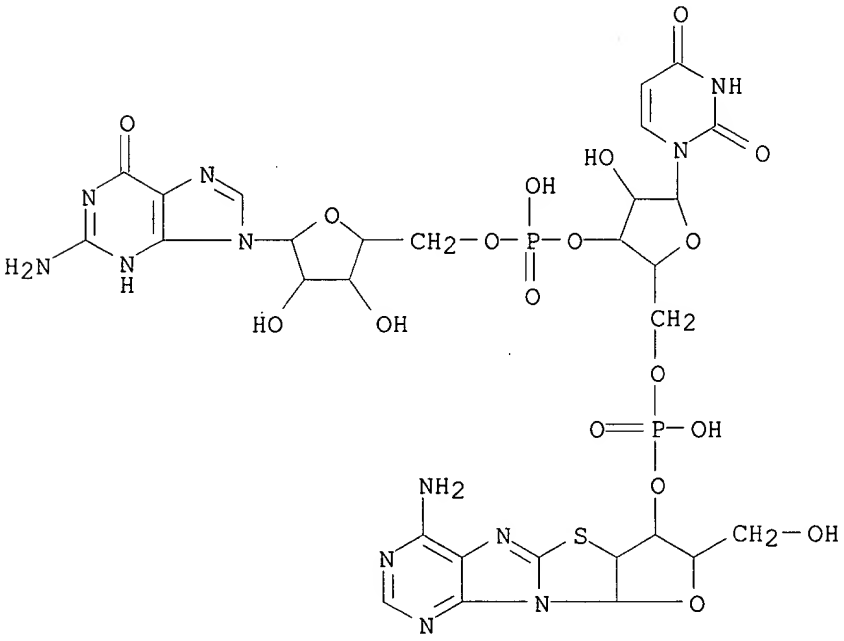


PAGE 2-A



RN 55048-89-0 HCAPLUS
CN Guanosine, 2'-deoxy-2',8-epithioadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)



RN 55196-42-4 HCAPLUS
CN Guanosine, 5'-deoxy-5',8-epithioadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

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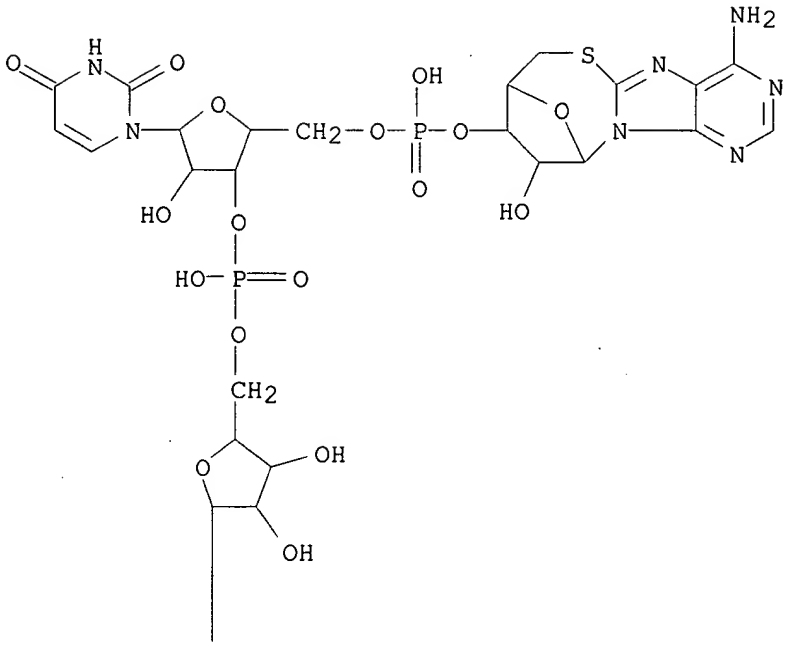

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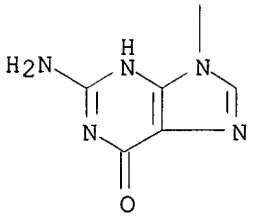

L8 ANSWER 77 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1975:58038 HCAPLUS
DOCUMENT NUMBER: 82:58038
TITLE: Polynucleotides. XXVI. Complex formation of polynucleotides derived from formycin and laurusin with cyclonucleoside oligonucleotides
AUTHOR(S): Ikehara, Morio; Tezuka, Toru
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Nucleic Acids Res. (1974), 1(7), 907-17
CODEN: NARHAD
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Poly(formycin phosphate) and poly(laurusin phosphate) were prepd. by polymg. formycin and laurusin 5'-diphosphate with E. coli polynucleotide phosphorylase. Poly(formycin phosphate) did not form the complex with an octanucleotide of 6,2'-anhydro-1-.beta.-D-arabino-furanosyluracil,

poly(laurusin phosphate) formed a 1:1 complex with octanucleotide of 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine in the presence of 0.15M Na ion at neutrality and 3.degree.. CD spectrum of this complex showed a couple of a trough at 286 nm and a peak at 262 nm., suggesting a left-handed helical conformation, which is opposite to the natural double helical polynucleotides.

IT **55132-83-7**
RL: RCT (Reactant)
(mixing curves and CD spectra in presence of sodium cacodylate)

RN 55132-83-7 HCAPLUS

CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-5'-O-phosphono-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio-, complex with 1,4-dihydro-3-(5-O-phosphono-.beta.-D-ribofuranosyl)-7H-pyrazolo[4,3-d]pyrimidin-7-one homopolymer (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 55132-82-6
CMF C80 H82 N40 O41 P8 S8
CDES *

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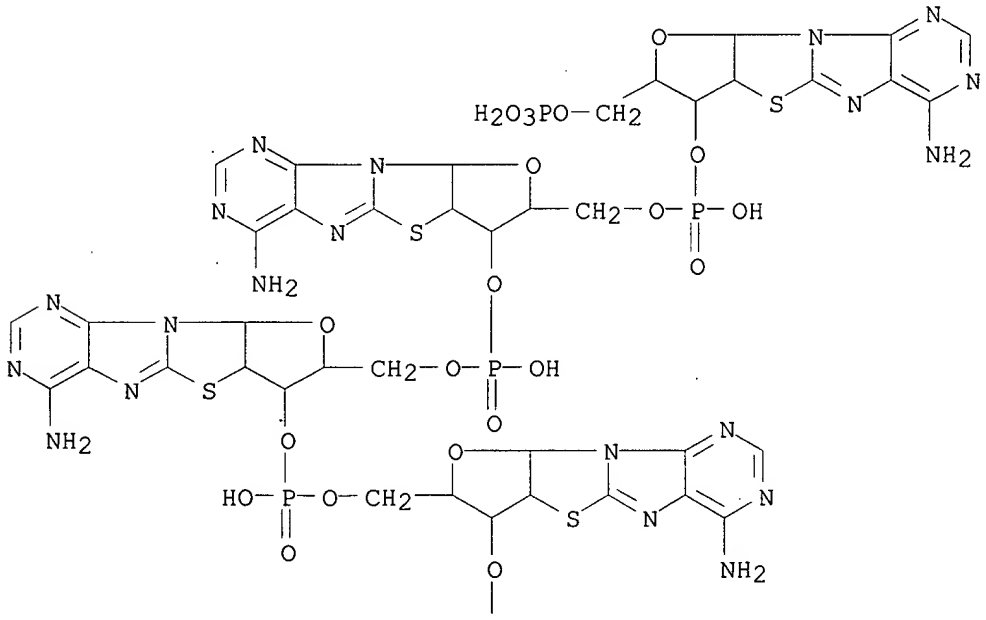
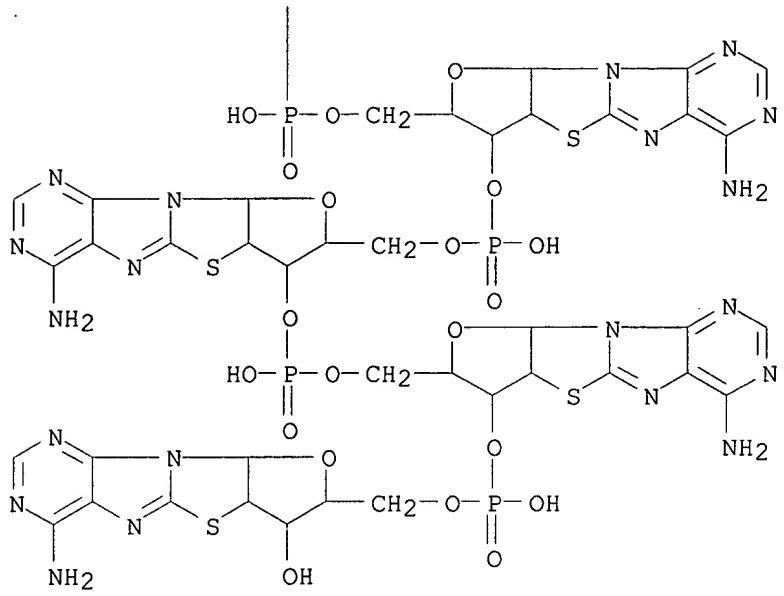




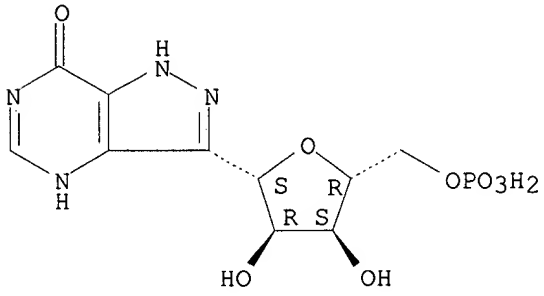
CM 2

CRN 55053-62-8
CMF (C10 H13 N4 O8 P)x
CCI PMS

CM 3

CRN 19495-11-5
CMF C10 H13 N4 O8 P
CDES 5:B-D-RIBO

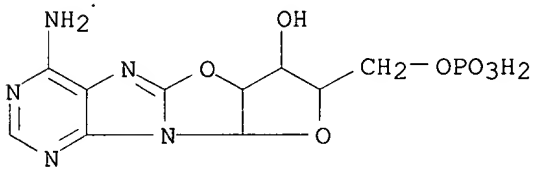
Absolute stereochemistry.



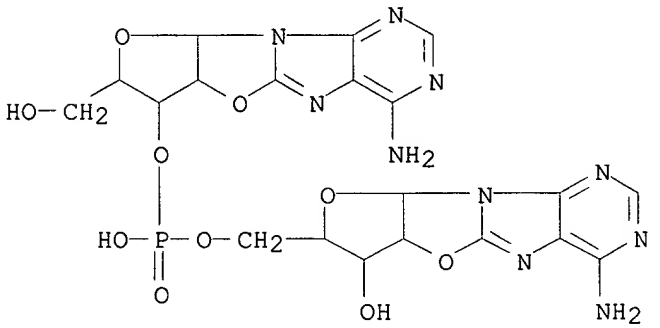
L8 ANSWER 78 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:491846 HCAPLUS
DOCUMENT NUMBER: 81:91846
TITLE: Polynucleotides. XXIV. Synthesis and properties of a dinucleoside monophosphate derived from 8,2'-O-cycloadenosine

AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi; Yano, Junichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Tayonaka, Japan
SOURCE: J. Amer. Chem. Soc. (1974), 96(15), 4966-72
CODEN: JACSAT
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The dinucleoside I was prepd. from 8,2'-anhydro-8-hydroxy-5'-(monomethoxytrityl)-9-.beta.-D-arabinofuranosyladenine and 8,2'-anhydro-N6,3'-diacetyl-8-hydroxy-9-.beta.-D-arabinofuranosyladenine using dicyclohexylcarbodiimide as the condensing reagent. The uv spectra taken under various conditions of temp. and salt concn. indicated that I had a well-stacked thermally stable conformation. CD spectra of I, having curves sym. reversed from those of usual ApA, suggest a stacking of two adenine moieties along the left-ApA, suggest a stacking of two adenine moieties along the left-handed screw axis, as was previously obsd. in S-cyclonucleoside oligomers.

IT **42735-42-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acetylation of)
RN 42735-42-2 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

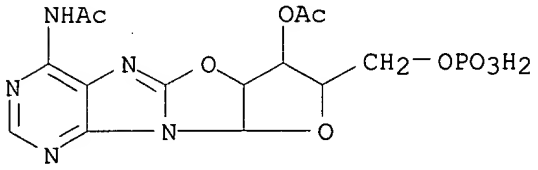


IT **39697-78-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and enzymatic hydrolysis of)
RN 39697-78-4 HCAPLUS
CN Adenosine, 2',8-anhydro-8-hydroxyadenylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)

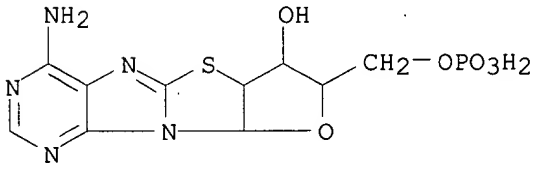


IT **52989-04-5**
RL: RCT (Reactant)
(reaction of, with cycloadenosines)
RN 52989-04-5 HCAPLUS

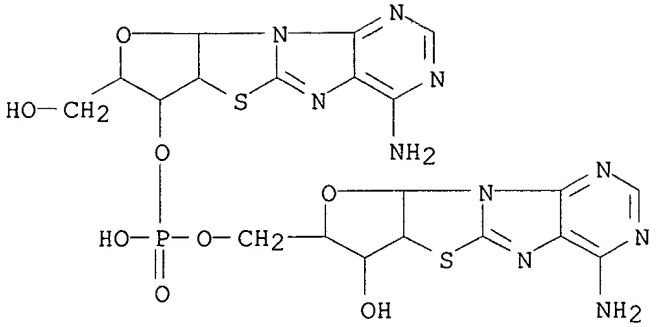
CN Acetamide, N-[7-(acetyloxy)-6a,7,8,9a-tetrahydro-8-[(phosphonooxy)methyl]furo[2',3':4,5]oxazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



L8 ANSWER 79 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:121253 HCAPLUS
DOCUMENT NUMBER: 80:121253
TITLE: Chemistry of purine 8-cyclonuclosides
AUTHOR(S): Ikehara, M.; Tada, H.
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: Jerusalem Symp. Quantum Chem. Biochem. (1972), 4, 455-68
CODEN: JSQCA7
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Anhydro- and thioanhydro- purine nucleosides were prepd. and their conformation detd. by uv, CD, ORD, and NMR studies.
IT **28220-14-6 29617-82-1 35837-07-1 52021-41-7**
RL: PRP (Properties)
(conformation of)
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



RN 29617-82-1 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



RN 35837-07-1 HCAPLUS
CN Diphosphoric acid, P,P'-bis[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-furo[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] ester, [6aR-[6a.alpha.,7.alpha.,8.beta.(6aR*,7S*,8S*,9aS*),9a.alpha.]]- (9CI) (CA INDEX NAME)

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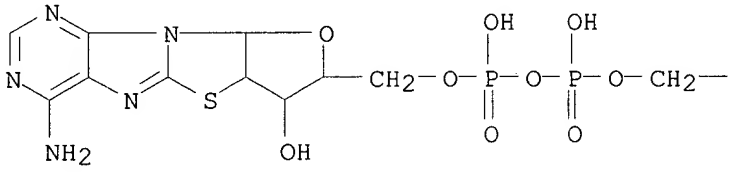

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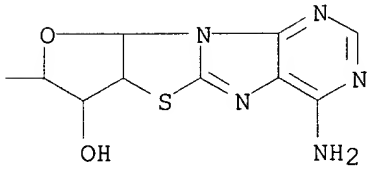
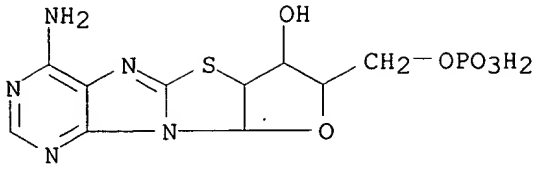


RN 52021-41-7 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 28220-14-6
CMF C10 H12 N5 O6 P S
CDES *

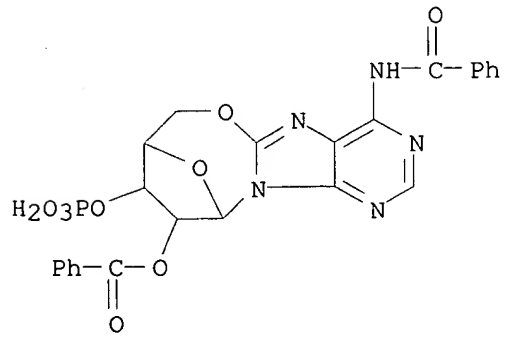


L8 ANSWER 80 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1974:96272 HCAPLUS
DOCUMENT NUMBER: 80:96272
TITLE: Polynucleotides. XX. Synthesis of an AUG analog containing 8,5'-o-cycloadenosine
AUTHOR(S): Ikehara, Morio; Nagura, Takeo; Ohtsuka, Eiko
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Chem. Pharm. Bull. (1974), 22(1), 123-7
CODEN: CPBTAL
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 8,5'-Anhydro-8-oxyadenosine was phosphorylated using cyanoethylphosphate and dicyclohexylcarbodiimide (DCC) in DMF-pyridine. Treatment of the products with a mixt. of 50% aq. pyridine-Et3N and DEAE-cellulose chromatog. gave 48% 2',3'-cyclic phosphate. 8,5'-Anhydro-8-oxyadenosine 3'-phosphate was obtained by RNase M digestion of the cyclic phosphate. After protection with benzoic anhydride in tetraethylammonium benzoate buffer, the 3'-phosphate was condensed with 2'-O-benzoyluridylyl-(3' .fwdarw. 5')-N2,2',3'-tri-O-isobutyrylguanosine by the use of DCC. DEAE-cellulose, Sephadex G-25 and G-15 column chromatog. gave 8,5'-anhydro-8-oxyadenylyl-(3' .fwdarw. 5')-uridylyl-(3' .fwdarw. 5')-guanosine, characterized by degrdn. to cyclo Ap, Up, and G with RNase M.

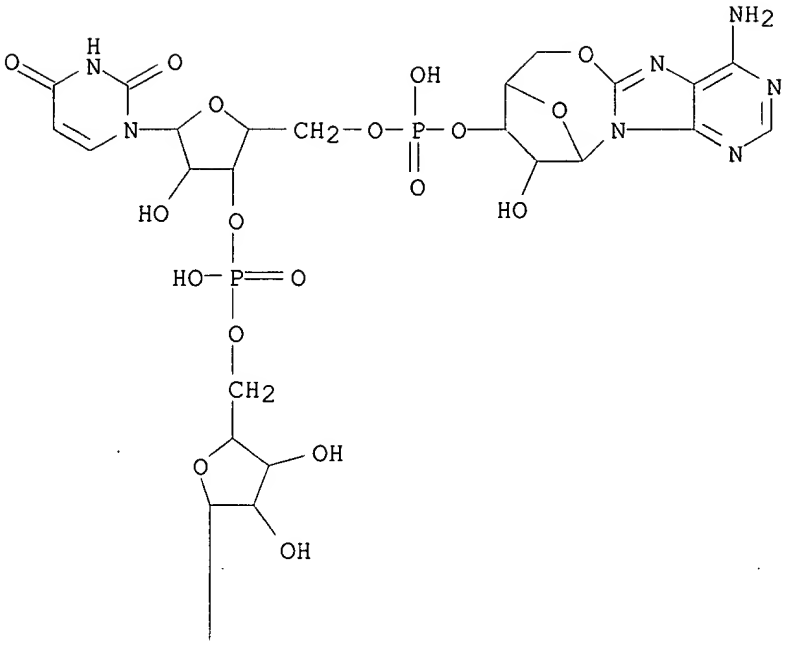
IT **52482-89-0P 52551-06-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 52482-89-0 HCAPLUS
CN Benzamide, N-[10-(benzoyloxy)-8,9,10,11-tetrahydro-9-(phosphonooxy)-8,11-epoxy-7H-[1,3]oxazocino[3,2-e]purin-4-yl]-, [8R-(8.alpha.,9.beta.,10.beta.,11.alpha.)]- (9CI) (CA INDEX NAME)

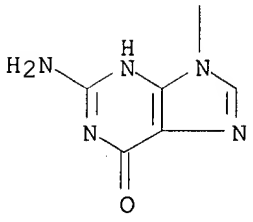


RN 52551-06-1 HCAPLUS
CN Guanosine, 5'-deoxy-5',8-epoxyadenylyl-(3'.fwdarw.5')-uridylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

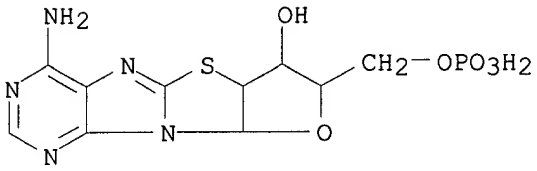


L8 ANSWER 81 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:492527 HCAPLUS
DOCUMENT NUMBER: 79:92527
TITLE: Anhydronucleosides. XI. Synthesis of nucleotides from 8,2'-thioanhydropurine nucleosides
AUTHOR(S): Ogilvie, Kelvin K.; Slotin, Lewis A.
CORPORATE SOURCE: Dep. Chem., Univ. Manitoba, Winnipeg, Manitoba, Can.
SOURCE: Can. J. Chem. (1973), 51(14), 2397-405
CODEN: CJCHAG
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The 5'-mono and diphosphates of the 8,2'-thioanhydropurine nucleosides were prepd. and studied with 5'-nucleotidase, alk. phosphatase, and adenylate kinase. Procedures for the prepn. of protected anhydronucleosides and their incorporation into dianhydronucleoside monophosphates were developed. These nucleotides were completely resistant to spleen and snake venom phosphodiesterases but were converted

with Raney Ni into the natural 2'-deoxynucleotides.

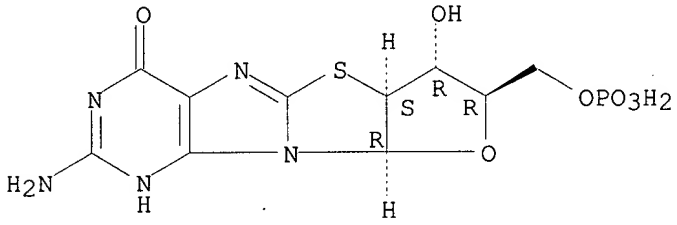
IT **28220-14-6P 50458-23-6P 50458-24-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with dephosphorylation enzymes)

RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



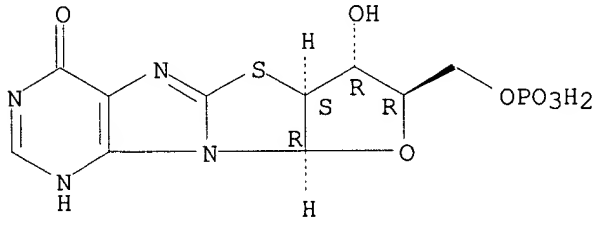
RN 50458-23-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purin-4(3H)-one, 2-amino-6a,7,8,9a-tetrahydro-7-hydroxy-8-[(phosphonooxy)methyl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



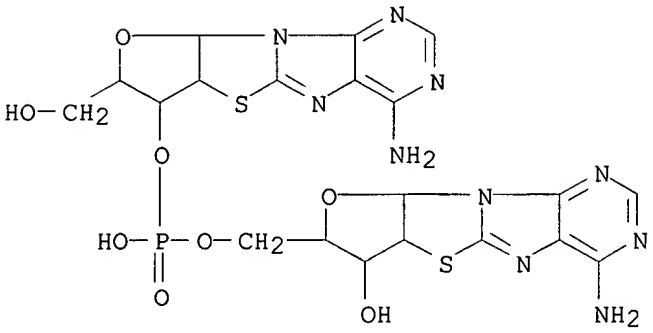
RN 50458-24-7 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purin-4(3H)-one, 6a,7,8,9a-tetrahydro-7-hydroxy-8-[(phosphonooxy)methyl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

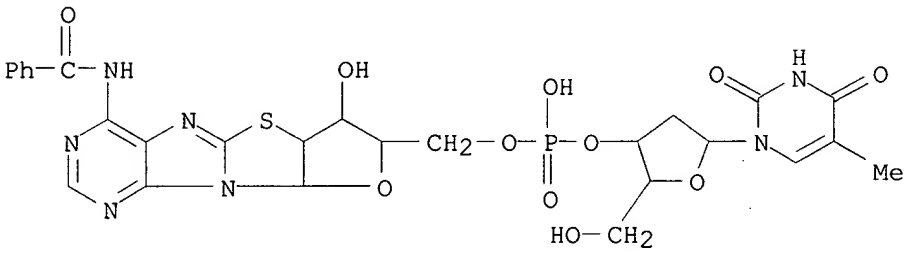


IT **29617-82-1P 50271-83-5P 50271-85-7P**
**50271-86-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

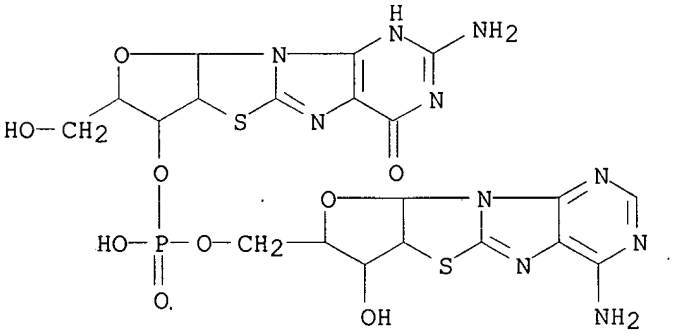
RN 29617-82-1 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



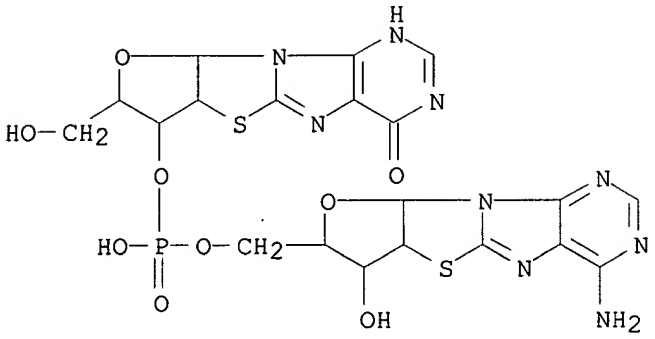
RN 50271-83-5 HCAPLUS
CN 3'-Thymidylic acid, mono[[4-(benzoylamino)-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



RN 50271-85-7 HCAPLUS
CN Phosphoric acid, mono[2-amino-1,4,6a,7,8,9a-hexahydro-8-(hydroxymethyl)-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-7-yl] mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] ester, stereoisomer (9CI) (CA INDEX NAME)

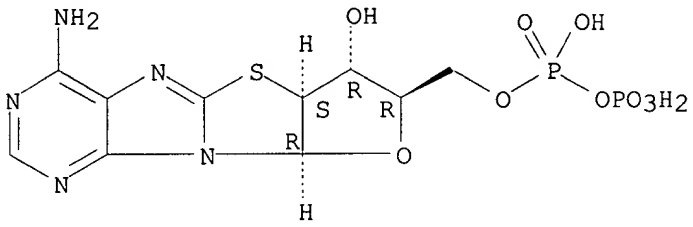


RN 50271-86-8 HCAPLUS
CN Phosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] mono[1,4,6a,7,8,9a-hexahydro-8-(hydroxymethyl)-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-7-yl] ester, stereoisomer (9CI) (CA INDEX NAME)



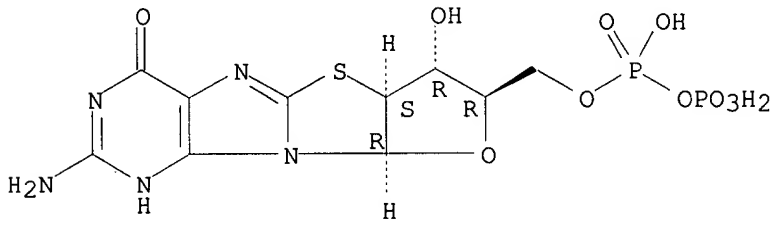
IT **42578-94-9P 50271-75-5P 50271-76-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and reaction with dephosphorylation enzymes)
RN 42578-94-9 HCAPLUS
CN Diphosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



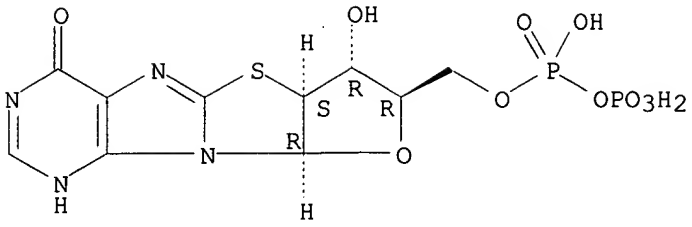
RN 50271-75-5 HCAPLUS
CN Diphosphoric acid, mono[[(6aS,7R,8R,9aR)-2-amino-1,4,6a,7,8,9a-hexahydro-7-hydroxy-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



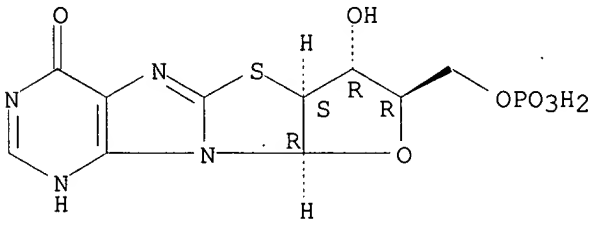
RN 50271-76-6 HCAPLUS
CN Diphosphoric acid, mono[[(6aS,7R,8R,9aR)-1,4,6a,7,8,9a-hexahydro-7-hydroxy-4-oxofuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl]methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 82 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:479110 HCAPLUS
DOCUMENT NUMBER: 79:79110
TITLE: Synthesis of 2'- and 3'-deoxyinosines
AUTHOR(S): Yamazaki, Akihiro; Akiyama, Masao; Kumashiro, Izumi; Ikehara, Morio
CORPORATE SOURCE: Cent. Res. Lab., Ajinomoto Co., Inc., Kawasaki, Japan
SOURCE: Chem. Pharm. Bull. (1973), 21(5), 1143-6
CODEN: CPBTAL
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Isopropylidenation of 8-mercaptoinosine with Me2C(OMe)2 in HClO4, followed by acetylation with Ac2O in pyridine, and then deisopropylidenation gave 5'-O-acetyl-8-mercaptoinosine (I). Tosylation of I, followed by treatment with NH3 in MeOH at 0.degree. gave 18% 8,2'-anhydro-8-mercapto-9-.beta.-D-arabino-(II) and 5.1% 8,3'-anhydro-8-mercapto-9-.beta.-D-xylofuranosylhypoxanthine (III). Refluxing II and III with Raney Ni in aq. soln. gave 2'-deoxy- and 3'-deoxyinosine, resp. Treatment of II with POCl3 in (MeO)3PO, followed by hydrolysis gave 8.5% of the 5'-phosphate ester of II.
IT **42926-62-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 42926-62-5 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purin-4(1H)-one, 6a,7,8,9a-tetrahydro-7-hydroxy-8-[(phosphonooxy)methyl]-, disodium salt, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 Na

L8 ANSWER 83 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:439643 HCAPLUS

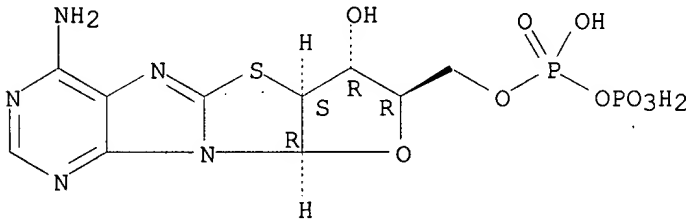
DOCUMENT NUMBER: 79:39643
TITLE: Polynucleotides. XVII. Effect of the diphosphates of aristeromycin and cycloadenosine on the polymerization of adenosine diphosphate by polynucleotide phosphorylase
AUTHOR(S): Ikehara, Morio; Fukui, Toshikazu
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: J. Biochem. (Tokyo) (1973), 73(5), 945-50
CODEN: JOBIAO
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Aristeromycin 5'-diphosphate (ArDP) and 2'-8anhydro-8-mercapto-9-.beta.-Darabinofuranosyladeninine 5'-diphosphate (cycloadenosine DP or ADP) were synthesized and tested for their properties in the polymn. catalyzed by Escherichia coli polynucleotide phosphorylase [E.C. 2.7.7.8]. AsDP was neither homopolymde. or copolymd. with ADP. However, it showed a stimulating effect in the polymn. of ADP to an extent of 30%. Therefore, a site other than that responsible for polymn. was involved in regulation of the reaction. ArDP was a poor substrate for polynucleotide phosphorylase and the extent of its homopolymn. was only 0.9%. ArDP was polymd. analyzed by alk. digestion to contain adenosine and aristeromycin residues radnomly. Uv and CD spectra of poly(A, Ar) were similar to those of poly(A).

IT **42578-94-9**
RL: BIOL (Biological study)
(polynucleotide phosphorylase polymn. of ADP in presence of)

RN 42578-94-9 HCAPLUS
CN Diphosphoric acid, mono[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxyfuro[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] ester, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



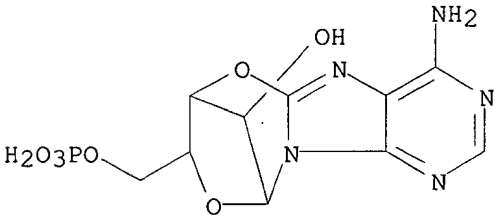

L8 ANSWER 84 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:428870 HCAPLUS
DOCUMENT NUMBER: 79:28870
TITLE: Substrate properties of 8,2'- and 8,3'-O-cyclo derivatives of adenosine 5'-monophosphate with adenosine 5'-monophosphate utilizing enzymes
AUTHOR(S): Hampton, Alexander; Sasaki, Takuma
CORPORATE SOURCE: Inst. Cancer Res., Philadelphia, Pa., USA
SOURCE: Biochemistry (1973), 12(12), 2188-91
CODEN: BICHAW
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The 5'-phosphates of 3'-deoxyadenosine, 9-.beta.-D-arabinofuranosyladenine, 8,2'-anhydro-8-hydroxy-9-.beta.-arabinofuranosyladenine, and 8,3'-anhydro-8-hydroxy-9-.beta.-D-xylofuranosyladenine were synthesized by phosphorylation of the

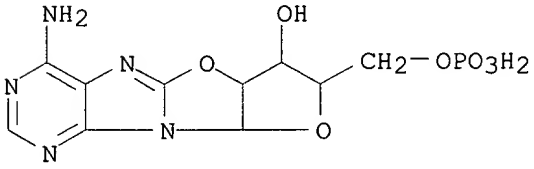
corresponding nucleosides and examd. together with the 5'-phosphates of 2'-deoxyadenosine and 9-.beta.-D-xylofuranosyladenine as substrates of rabbit adenosine 5'-phosphate (AMP) aminohydrolase, snake venom 5'-nucleotidase, and rabbit AMP kinase. The resp. Vmax values of the 8,2'- and 8,3'-cyclonucleotides relative to AMP were 0.85 and 0.55% with 5'-nucleotidase, 0.008 and <0.001% (AMP aminohydrolase), and 0.057 and 0.045% (AMP kinase). These findings, together with the substrate properties of the remaining compds. and addnl. substrate specificity characteristics of the enzymes, accord with a previous conclusion that the adenine-ribose torsion angle of enzyme-bound AMP is such that H-8 is oriented in the vicinity of C-4'.

IT **42582-26-3 42735-42-2**
RL: BIOL (Biological study)
(as AMP-metabolizing enzymes substrates)

RN 42582-26-3 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]dioxazepino[3,2-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12R*)]- (9CI) (CA INDEX NAME)




RN 42735-42-2 HCAPLUS
CN Furo[2',3':4,5]oxazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)




L8 ANSWER 85 OF 94 HCAPLUS COPYRIGHT 2002 ACS

| | |
|---|---|
| ACCESSION NUMBER: | 1973:107536 HCAPLUS |
| DOCUMENT NUMBER: | 78:107536 |
| TITLE: | Evidence for the conformation of enzyme-bound adenosine 5'-phosphate. Substrate and inhibitor properties of 8,5'-cycloadenosine 5'-phosphate with adenylate kinase, adenylate aminohydrolase, adenylosuccinate lyase, and 5'-nucleotidase |
| AUTHOR(S): | Hampton, Alexander; Harper, Peter J.; Sasaki, Takuma |
| CORPORATE SOURCE: | Inst. Cancer Res., Philadelphia, Pa., USA |
| SOURCE: | Biochemistry (1972), 11(26), 4965-9<br>CODEN: BICHAW |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |

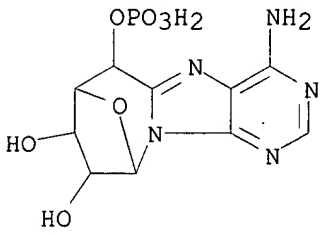
GI For diagram(s), see printed CA Issue.

AB Phosphorylation of 2',3'-O-isopropylidene-8,5'-cycloadenosine followed by removal of the isopropylidene group and furnished 8,5'-cycloadenosine 5'-phosphate (8,5'-cyclo-AMP) (I) as a 1:3 ratio of 5' epimers of which only the minor one was a substrate of venom 5'-nucleotidase and pig muscle AMP kinase. With AMP aminohydrolase of rabbit muscle the epimeric mixt. gave essentially the same Vmax as AMP and a Km of 2.0mM (AMP, Vmax = 1140 .mu.moles/min per mg protein; Km = 0.3mM). With snake venom 5 -nucleotidase, Vmax of the active epimer (0.5-0.75 .mu.moles/min per mg protein) was comparable to that of AMP (1.25 .mu.moles/min per mg of protein). With AMP kinase, 8,5'-cyclo-AMP reacted twice as rapidly as the same level (1.25.mu.M) of AMP. The 8,5'-cyclo-ADP so produced was a substrate of rabbit muscle pyruvate kinase. These data together with evidence that the phosphate moiety, the furanose ring, and the adenine ring of AMP all are required for or promote catalytic efficiency, indicate that enzyme-bound AMP probably possesses a sugas-base torsion angle similar to that of 8,5'-cyclo-AMP, and that the 5'-oxygen of AMP is most likely oriented in a direction between H-3' and H-4'. 8,5'-Cyclo-AMP was a strong competitive inhibitor of AMP aminohydrolase (apparent Ki = 55.mu.M; Km (for AMP) = 0.3mM) and of the conversion of adenylosuccinate to AMP by Escherichia coli adenylosuccinate lyase (Ki = 8.mu.M; Ki (for AMP) = 13.mu.M), suggesting that in aq. soln. the conformation of AMP may resemble that postulated for enzyme-bound AMP. Thus catalytic conversion of AMP by the above three enzymes is unlikely to be accompanied by significant rotation about the 4',5' and glycosidic bonds or puckering of the ribofuranose ring of AMP.

IT **41036-59-3**
RL: BIOL (Biological study)
(enzyme response to)

RN 41036-59-3 HCAPLUS

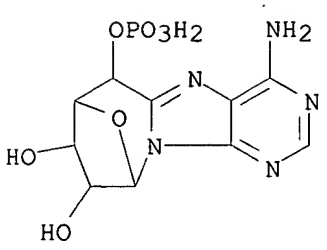
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6S-(6.alpha.,7.beta.,8.beta.,9.beta.,10.beta.)]- (9CI) (CA INDEX NAME)




IT **41116-92-1**
RL: BIOL (Biological study)
(enzymes response to)

RN 41116-92-1 HCAPLUS

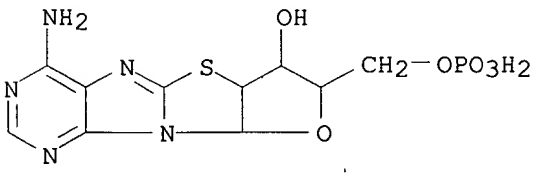
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate), [6R-(6.alpha.,7.alpha.,8.alpha.,9.alpha.,10.alpha.)]- (9CI) (CA INDEX NAME)



L8 ANSWER 86 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:72504 HCAPLUS
DOCUMENT NUMBER: 78:72504
TITLE: Polynucleotides. XVI. Oligomers of 8,2'-anhydro-8-mercapto-9-(.beta.-D-arabinofuranosyl)adenine 5'-monophosphate
AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: J. Amer. Chem. Soc. (1972), 94(26), 9189-23
CODEN: JACSAT
DOCUMENT TYPE: Journal
LANGUAGE: English

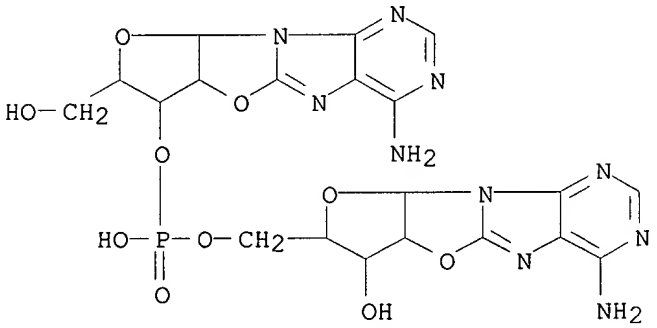
AB N6-Benzoyl-8,2'-anhydro-8-mercapto-9-(.beta.-D-arabinofuranosyl)adenine 5'-phosphate was subjected to polymerization using dicyclohexylcarbodiimide in pyridine. The resulting polynucleotides (pAs)n were isolated and purified by means of DEAE-cellulose column chromatog., paper chromatog., and paper electrophoresis. Chain lengths were obtained by phosphate anal. of the polymer and its dephosphorylated product formed by alk. phosphatase digest. All these polynucleotides had CD spectra of similar profile, which had a trough at 277-288 nm and two peaks at around 264 and 222 nm, resp. Based on the similarity of these spectra with that of AspAs previously obtained, the same conformations were assigned to the polymers, i.e., stacked with a left-handed screw axis. The magnitude of Cotton effect [.theta.] and uv absorbance increased with increasing chain length and reached a plateau at five to six nucleotide units. While [.theta.] of the pentamer decreased to 62% from 0 to 80.degree., extinction coefficient decreased only 15% from 10 to 90.degree..

IT **28220-14-6**
RL: RCT (Reactant)
(benzoylation of)
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



L8 ANSWER 87 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1973:43911 HCAPLUS

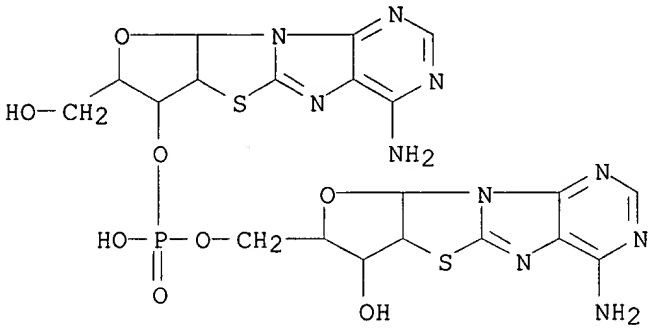
DOCUMENT NUMBER: 78:43911
TITLE: Left-handed helical polynucleotides with D-sugar phosphodiester backbones
AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi; Yano, Junichi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: Nature (London), New Biol. (1972), 240(96), 16-17
CODEN: NNBYA7
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB A dinucleoside monophosphate with a structure (Ib) similar to previously prepd. (Ia) was synthesized. It is 8,2'-anhydro-8-oxy-9-.beta.-D-arabinofuranosyladenine phosphoryl-(3' .fwdarw. 5')-8,-2'-anhydro-8-oxy-9-.beta.-D-arabinofuranosyladenine (A.degree.pA.degree.). Polynucleotides in which 3-10 As residues were linked, were also synthesized and their conformation and thermal stabilities studied. Ib was synthesized from the corresponding anhydronucleosides by phosphorylation of 1 unit and condensation with another protected anhydronucleoside. It was established that the new compd. must be left-handed.
IT **39697-78-4**
RL: PRP (Properties)
(structure of)
RN 39697-78-4 HCAPLUS
CN Adenosine, 2',8-anhydro-8-hydroxyadenylyl-(3'.fwdarw.5')-2',8-anhydro-8-hydroxy- (9CI) (CA INDEX NAME)



L8 ANSWER 88 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1972:502112 HCAPLUS
DOCUMENT NUMBER: 77:102112
TITLE: Synthesis and properties of the dinucleoside monophosphate of adenine 8-thiocyclonucleoside
AUTHOR(S): Uesugi, Seiichi; Yasumoto, Mitsugu; Ikehara, Morio; Fang, Kai N.; Ts'o, Paul O. P.
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: J. Amer. Chem. Soc. (1972), 94(15), 5480-6
CODEN: JACSAT
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The dinucleoside monophosphate (AspAs) of 8,2'-anhydro-8-mercapto-9-(.beta.-D-arabinofuranosyl)adenine was synthesized, and its properties investigated by uv absorption, CD, and PMR. Comparison was made with diadenosine monophosphate (ApA) in these properties. The results indicate that the conformation of AspAs has two special characteristics: (1) it is a left-handed stack with considerable base-base overlap, and (2) it is

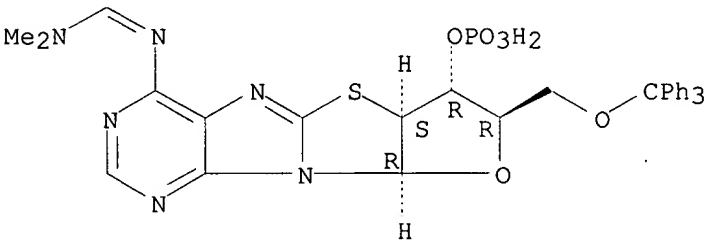
relatively stable against thermal perturbation. Also, AspAs is very resistant to both venom and spleen phosphodiesterases and does not form a complex with poly U.

IT **29617-82-1**
RL: PRP (Properties)
(conformation of, NMR, CD and uv spectra in relation to)
RN 29617-82-1 HCAPLUS
CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



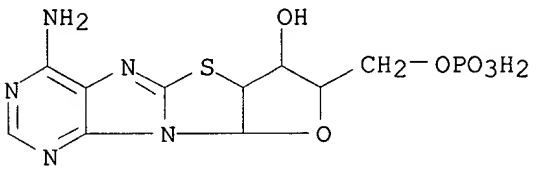
IT **38934-65-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 38934-65-5 HCAPLUS
CN Methanimidamide, N,N-dimethyl-N'-[6a,7,8,9a-tetrahydro-7-(phosphonooxy)-8-[(triphenylmethoxy)methyl]furo[2',3':4,5]thiazolo[3,2-e]purin-4-yl]-, [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

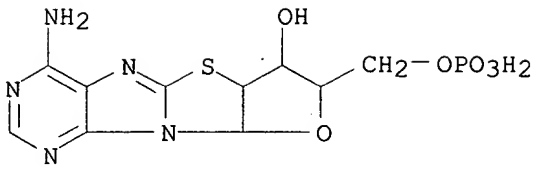


L8 ANSWER 89 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1972:475399 HCAPLUS
DOCUMENT NUMBER: 77:75399
TITLE: Nucleosides and nucleotides. LIII. Purine cyclonucleosides-18. Selective tosylation of adenine nucleotides. Synthesis of 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine 5'-and 3',5-cyclic phosphate
AUTHOR(S): Ikehara, M.; Uesugi, S.
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
SOURCE: Tetrahedron (1972), 28(14), 3687-94
CODEN: TETRAB

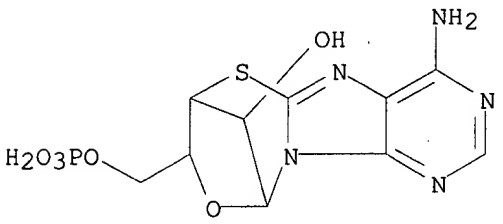
DOCUMENT TYPE: Journal
LANGUAGE: English
AB AMP and AMP 8-bromo were treated with tosyl chloride in aq. alk. soln. to give 2'-tosyl nucleotides. AMP 8-bromo-2'-tosyl deriv. was cyclized to 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine (I) 5'-monophosphate (II) by treatment with H2S in pyridine or NaSH in aq. DMF. Desulfurization of II gave AMP 2'-deoxy analog. Adenosine 3',5'-cyclic phosphate 8-bromo deriv. was similarly tosylated and cyclized to give I 3',5'-cyclic phosphate. Snake venom 5'-nucleotidase and Escherichia coli and sheep-intestine alkaline phosphatases hydrolyzed II to give 8,2'-S-cyclo nucleosides.
IT **28220-14-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)




L8 ANSWER 90 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1972:113482 HCAPLUS
DOCUMENT NUMBER: 76:113482
TITLE: Nucleosides and nucleotides. XLVII. Conformation of purine mucleosides and their 5'-phosphates
AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi; Yoshida, Katsumi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Biochemistry (1972), 11(5), 830-6
CODEN: BICHAW
DOCUMENT TYPE: Journal
LANGUAGE: English
AB CD of purine nucleosides and their 5'-monophosphates was measured. From the relative rotational strength and sign of the Cotton effect the following conclusions were reached. Purine nucleosides having bulky substituents in the 8 position, such as Br, 2-hydroxypropyl, and MeS group, have syn conformations. Introduction of a phosphate to the 5'-hydroxyl group of anti-type nucleosides, such as adenosine, 8,2'-and 8,3'-S-cycloadenosine, does not change the CD curve in the B-band region. Introduction of a phosphate to the 5'-hydroxyl group of syn-type nucleosides such as 8-substituted purine nucleosides caused a drastic change of CD curves over a wide range of wavelength. Both in syn- and anti-type purine nucleosides, introduction of the 5'-phosphate caused a significant change in the Cotton band at 200-220 nm.
IT **28220-14-6 35782-70-8**
RL: PRP (Properties)
(CD and uv spectra of, conformation in relation to)
RN 28220-14-6 HCAPLUS
CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



RN 35782-70-8 HCAPLUS
CN 7,10-Methano-10H-[1,5,3]oxathiazepino[3,4-e]purine-8-methanol, 4-amino-7,8-dihydro-12-hydroxy-, .alpha.-(dihydrogen phosphate), [7R-(7.alpha.,8.beta.,10.alpha.,12S*)]- (9CI) (CA INDEX NAME)

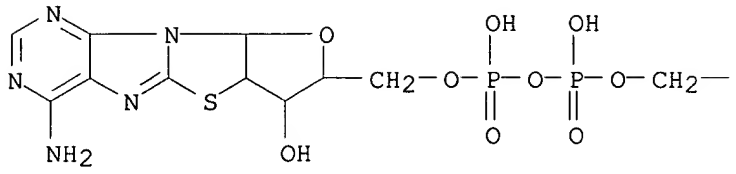


L8 ANSWER 91 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1972:113475 HCAPLUS
DOCUMENT NUMBER: 76:113475
TITLE: Nucleosides and nucleotides. XLVIII. Conformation of purine nucleoside pyrophosphates as studies by circular dichroism
AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi; Yoshida, Katsumi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: Biochemistry (1972), 11(5), 836-42
CODEN: BICHAW
DOCUMENT TYPE: Journal
LANGUAGE: English

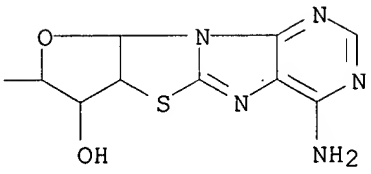
AB The CD of dinucleoside 5',5'-pyrophosphates of purine nucleosides was studied for elucidation of the conformation. Pyrophosphates derived from adenosine, inosine, guanosine, and 8,3'-S-cycloadenosine have a stacked sym. structure, in which bases are in anti conformation. 8,2'-S-Cycloadenosine 5',5'-pyrophosphate cannot have a stacked conformation due to the restricted rotation of the bases. Pyrophosphates from 8-bromoadenosine, as well as 8-bromoguanosine, have a stacked conformation, in which bases are in syn form.

IT **35837-07-1 35837-34-4**
RL: PRP (Properties)
(CD and uv spectra of, conformation in relation to)
RN 35837-07-1 HCAPLUS
CN Diphosphoric acid, P,P'-bis[(4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-furo[2',3':4,5]thiazolo[3,2-e]purin-8-yl)methyl] ester, [6aR-[6a.alpha.,7.alpha.,8.beta.(6aR*,7S*,8S*,9aS*),9a.alpha.]]- (9CI) (CA INDEX NAME)

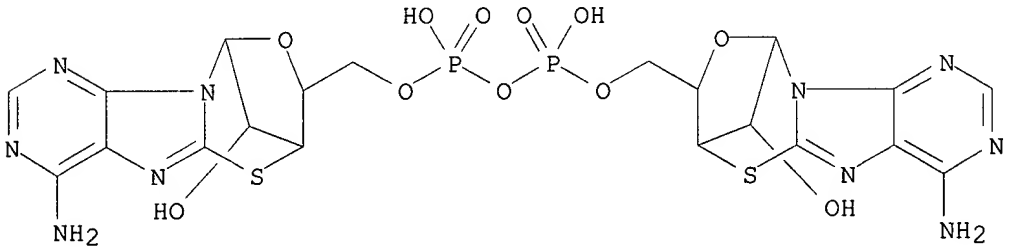
PAGE 1-A



PAGE 1-B



RN 35837-34-4 HCAPLUS
CN Diphosphoric acid, P,P'-bis[(4-amino-7,8-dihydro-12-hydroxy-7,10-methano-10H-[1,5,3]oxathiazepino[3,4-e]purin-8-yl)methyl] ester, [7R-[7.alpha.,8.beta.(7R*,8R*,10R*,12S*),10.alpha.,12S*]]- (9CI) (CA INDEX NAME)



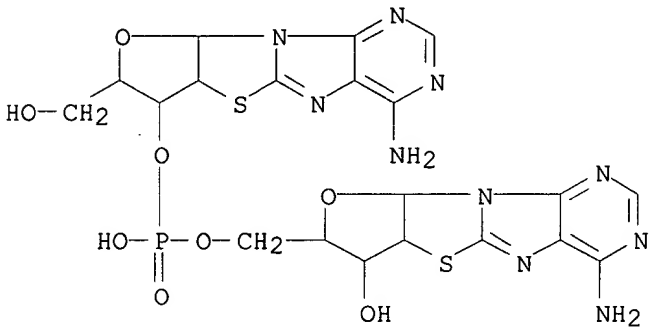
L8 ANSWER 92 OF 94 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1970:510043 HCAPLUS
DOCUMENT NUMBER: 73:110043
TITLE: Highly stacked dinucleoside monophosphate derived from adenine 8-cyclonucleosides
AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi; Yasumoto, Mitsugi
CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Toyonaka, Japan
SOURCE: J. Amer. Chem. Soc. (1970), 92(15), 4735-6
CODEN: JACSAT
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB I was synthesized from 8,2'-anhydro-N6-dimethylaminomethylene-5'-O-trityl-(9-.beta.-D- arabinofuranosyladenine) 3'-phosphate and 8,2'-anhydro-N6,O2-dibenzoyl-8-mercapto-9-.beta.-D-arabinofuranosyladenine by using dicyclohexylcarbodiimide as a condensing agent, followed by removal of the protecting groups. I showed an unusually strong stacking of the adenine ring, and formed a left-handed helical structure opposite

to the right-handed one in adenylyl-(3' .fwdarw. 5')-adenosine.

IT **29617-82-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 29617-82-1 HCAPLUS

CN .beta.-D-arabino-Adenosine, 2'-deoxy-2',8-epithio-.beta.-D-arabino-adenylyl-(3'.fwdarw.5')-2'-deoxy-2',8-epithio- (9CI) (CA INDEX NAME)



L8 ANSWER 93 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:133127 HCAPLUS

DOCUMENT NUMBER: 72:133127

TITLE: Selective tosylation of adenosine 5'-monophosphate

AUTHOR(S): Ikehara, Morio; Uesugi, Seiichi

CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan

SOURCE: Tetrahedron Lett. (1970), (10), 713-16
CODEN: TELEAY

DOCUMENT TYPE: Journal

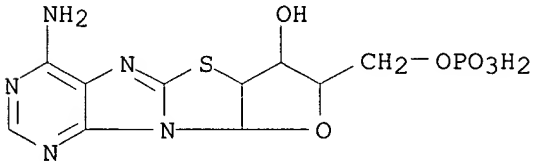
LANGUAGE: English

AB AMP was tosylated in position 2 of the sugar, followed by bromination in the position 8 of the purine and by treatment with NaSH to give 8,2'-anhydro-8-mercapto-9-.beta.-D-arabinofuranosyladenine 5'-monophosphate, which was converted into 2'-deoxyadenosine phosphate.

IT **28220-14-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 28220-14-6 HCAPLUS

CN Furo[2',3':4,5]thiazolo[3,2-e]purine-8-methanol, 4-amino-6a,7,8,9a-tetrahydro-7-hydroxy-, .alpha.-(dihydrogen phosphate), [6aS-(6a.alpha.,7.alpha.,8.beta.,9a.alpha.)]- (9CI) (CA INDEX NAME)



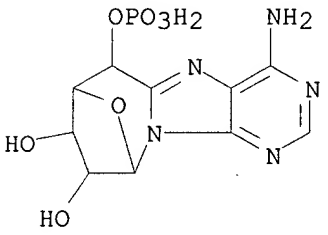
L8 ANSWER 94 OF 94 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1968:493478 HCAPLUS

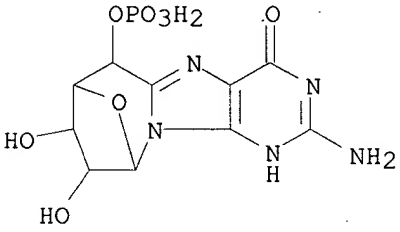
DOCUMENT NUMBER: 69:93478

TITLE: Cyclic nucleotide formation by irradiation of aqueous

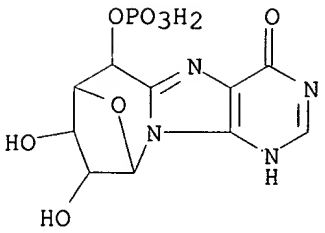
purine nucleotide solutions
AUTHOR(S): Keck, K.
CORPORATE SOURCE: Univ. Freiburg/Br., Freiburg/Br., Ger.
SOURCE: Z. Naturforsch., B (1968), 23(8), 1034-43
CODEN: ZENBAX
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The products of .gamma.- or x-irradn. of O-free solns. of AMP were sepd. by anion-exchange resins into 5 fractions, one of which contained the 8,5'-cyclonucleotide, I, .lambda. 635 m.mu.. Degradation of I by successive treatment with NaIO4, NaBH4, acid hydrolysis, and NaIO4 gave 8-formyladenine. This was reduced to 8-(hydroxymethyl)adenine and oxidized to 8-carboxyadenine, all compds. being identified by uv and thin-layer chromatog. IMP and GMP gave similar cyclic nucleotides. The N.M.R. spectrum of I in D2O was given, as well as the uv spectra of I, the N-oxide of I, and a P-contg. hydrolysis product of I.
IT **21082-64-4**
RL: FORM (Formation, nonpreparative)
(formation of, by radiolysis of 5'-adenylic acid)
RN 21082-64-4 HCAPLUS
CN 7,10-Epoxy-6H-azepino[1,2-e]purine-6,8,9-triol, 4-amino-7,8,9,10-tetrahydro-, 6-(dihydrogen phosphate) (8CI, 9CI) (CA INDEX NAME)




IT **21082-66-6**
RL: FORM (Formation, nonpreparative)
(formation of, by radiolysis of 5'-guanylic acid)
RN 21082-66-6 HCAPLUS
CN 7,10-Epoxy-4H-azepino[1,2-e]purin-4-one, 2-amino-3,6,7,8,9,10-hexahydro-6,8,9-trihydroxy-, 6-(dihydrogen phosphate) (8CI) (CA INDEX NAME)




IT **21082-65-5**
RL: FORM (Formation, nonpreparative)
(formation of, by radiolysis of 5'-inosinic acid)
RN 21082-65-5 HCAPLUS
CN 7,10-Epoxy-4H-azepino[1,2-e]purin-4-one, 3,6,7,8,9,10-hexahydro-6,8,9-trihydroxy-, 6-(dihydrogen phosphate) (8CI) (CA INDEX NAME)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